



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:39 PM UTC

PDB ID : 5COD / pdb_00005cod
Title : Bovine heart complex I membrane domain
Authors : Zhu, J.; Hirst, J.; King, M.S.; Yu, M.; Leslie, A.G.W.; Klipcan, L.
Deposited on : 2015-07-20
Resolution : 6.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

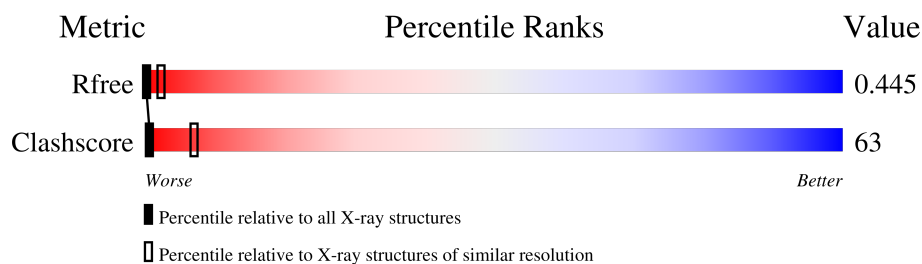
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



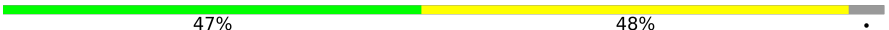









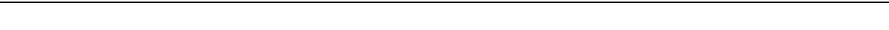

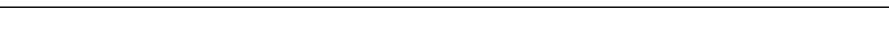
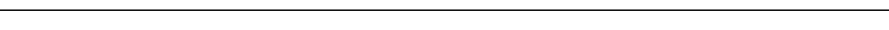











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1163 (9.44-4.00)
Clashscore	190562	1003 (9.44-4.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L1	606	
1	L2	606	
1	L3	606	
1	L4	606	
1	L5	606	
1	L6	606	
2	M1	459	
2	M2	459	
2	M3	459	


























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Mol	Chain	Length	Quality of chain
2	M4	459	
2	M5	459	
2	M6	459	
3	f1	30	
3	f2	30	
3	f3	30	
3	f4	30	
3	f5	30	
3	f6	30	
3	h1	30	
3	h2	30	
3	h3	30	
3	h4	30	
3	h5	30	
3	h6	30	
3	i1	30	
3	i2	30	
3	i3	30	
3	i4	30	
3	i5	30	
3	i6	30	
4	g1	22	
4	g2	22	
4	g3	22	
4	g4	22	












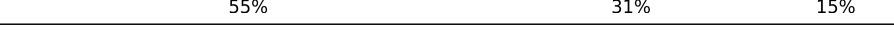







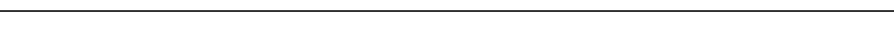

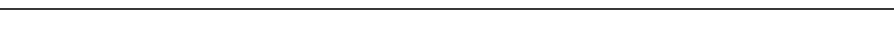
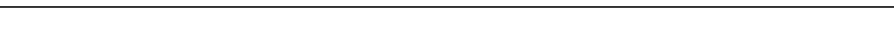


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Mol	Chain	Length	Quality of chain
4	g5	22	 45% 55%
4	g6	22	 55% 45%
5	j1	28	 68% 32%
5	j2	28	 68% 32%
5	j3	28	 68% 32%
5	j4	28	 68% 32%
5	j5	28	 68% 32%
5	j6	28	 68% 32%
5	k1	28	 82% 18%
5	k2	28	 82% 18%
5	k3	28	 82% 18%
5	k4	28	 82% 18%
5	k5	28	 82% 18%
5	k6	28	 82% 18%
5	p1	28	 79% 21%
5	p2	28	 79% 21%
5	p3	28	 79% 21%
5	p4	28	 79% 21%
5	p5	28	 79% 21%
5	p6	28	 79% 21%
5	s1	28	 61% 39%
5	s2	28	 61% 39%
5	s3	28	 57% 43%
5	s4	28	 57% 43%
5	s5	28	 57% 43%












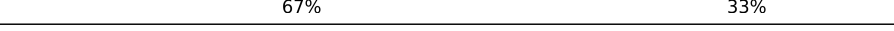







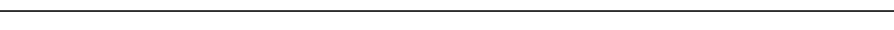

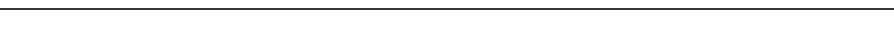
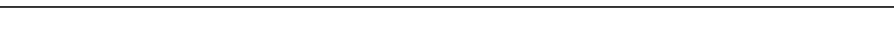


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Mol	Chain	Length	Quality of chain
5	s6	28	 61% 39%
6	l1	13	 54% 46%
6	l2	13	 54% 46%
6	l3	13	 54% 46%
6	l4	13	 54% 46%
6	l5	13	 54% 46%
6	l6	13	 69% 31%
7	U1	88	 55% 31% 15%
7	U2	88	 57% 28% 15%
7	U3	88	 55% 31% 15%
7	U4	88	 57% 28% 15%
7	U5	88	 55% 31% 15%
7	U6	88	 57% 28% 15%
8	n1	59	 56% 44%
8	n2	59	 56% 44%
8	n3	59	 56% 44%
8	n4	59	 53% 47%
8	n5	59	 53% 47%
8	n6	59	 58% 42%
9	o1	21	 100%
9	o2	21	 100%
9	o3	21	 100%
9	o4	21	 100%
9	o5	21	 100%
9	o6	21	 100%


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Mol	Chain	Length	Quality of chain
10	t1	57	 54% 46%
10	t2	57	 56% 44%
10	t3	57	 53% 47%
10	t4	57	 54% 46%
10	t5	57	 56% 44%
10	t6	57	 56% 44%
11	u1	15	 67% 33%
11	u2	15	 80% 20%
11	u3	15	 67% 33%
11	u4	15	 67% 33%
11	u5	15	 67% 33%
11	u6	15	 67% 33%
12	v1	32	 53% 47%
12	v2	32	 53% 47%
12	v3	32	 53% 47%
12	v4	32	 53% 47%
12	v5	32	 53% 47%
12	v6	32	 53% 47%
13	w1	27	 74% 26%
13	w2	27	 74% 26%
13	w3	27	 74% 26%
13	w4	27	 74% 26%
13	w5	27	 74% 26%
13	w6	27	 74% 26%
14	BA	146	 85% 14% •

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Mol	Chain	Length	Quality of chain
14	BB	146	 86% 13% .
14	BC	146	 84% 15% .
14	BD	146	 84% 15% .
14	BE	146	 83% 16% .
14	BF	146	 86% 14% .

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 48030 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	L1	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L2	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L3	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L4	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L5	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L6	493	Total	C	N	O	0	0	0
			2465	1479	493	493			

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M1	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M2	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M3	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M4	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M5	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M6	439	Total	C	N	O	0	0	0
			2195	1317	439	439			

- Molecule 3 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	f1	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	h1	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	i1	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	f2	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	h2	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	i2	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	f3	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	h3	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	i3	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	f4	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	h4	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	i4	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	f5	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	h5	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	i5	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	f6	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	h6	30	Total	C	N	O	0	0	0
			150	90	30	30			
3	i6	30	Total	C	N	O	0	0	0
			150	90	30	30			

- Molecule 4 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	g1	22	Total	C	N	O	0	0	0
			110	66	22	22			
4	g2	22	Total	C	N	O	0	0	0
			110	66	22	22			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	g3	22	Total	C	N	O	0	0	0
			110	66	22	22			
4	g4	22	Total	C	N	O	0	0	0
			110	66	22	22			
4	g5	22	Total	C	N	O	0	0	0
			110	66	22	22			
4	g6	22	Total	C	N	O	0	0	0
			110	66	22	22			

- Molecule 5 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	j1	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k1	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p1	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s1	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j2	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k2	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p2	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s2	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j3	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k3	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p3	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s3	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j4	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k4	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p4	28	Total	C	N	O	0	0	0
			140	84	28	28			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	s4	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j5	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k5	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p5	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s5	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j6	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k6	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p6	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s6	28	Total	C	N	O	0	0	0
			140	84	28	28			

- Molecule 6 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	l1	13	Total	C	N	O	0	0	0
			65	39	13	13			
6	l2	13	Total	C	N	O	0	0	0
			65	39	13	13			
6	l3	13	Total	C	N	O	0	0	0
			65	39	13	13			
6	l4	13	Total	C	N	O	0	0	0
			65	39	13	13			
6	l5	13	Total	C	N	O	0	0	0
			65	39	13	13			
6	l6	13	Total	C	N	O	0	0	0
			65	39	13	13			

- Molecule 7 is a protein called SDAP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	U1	75	Total	C	N	O	0	0	0
			375	225	75	75			
7	U2	75	Total	C	N	O	0	0	0
			375	225	75	75			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	U3	75	Total	C	N	O	0	0	0
			375	225	75	75			
7	U4	75	Total	C	N	O	0	0	0
			375	225	75	75			
7	U5	75	Total	C	N	O	0	0	0
			375	225	75	75			
7	U6	75	Total	C	N	O	0	0	0
			375	225	75	75			

- Molecule 8 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	n1	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n2	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n3	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n4	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n5	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n6	59	Total	C	N	O	0	0	0
			295	177	59	59			

- Molecule 9 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	o1	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o2	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o3	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o4	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o5	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o6	21	Total	C	N	O	0	0	0
			105	63	21	21			

- Molecule 10 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	t1	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t2	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t3	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t4	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t5	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t6	57	Total	C	N	O	0	0	0
			285	171	57	57			

- Molecule 11 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	u1	15	Total	C	N	O	0	0	0
			75	45	15	15			
11	u2	15	Total	C	N	O	0	0	0
			75	45	15	15			
11	u3	15	Total	C	N	O	0	0	0
			75	45	15	15			
11	u4	15	Total	C	N	O	0	0	0
			75	45	15	15			
11	u5	15	Total	C	N	O	0	0	0
			75	45	15	15			
11	u6	15	Total	C	N	O	0	0	0
			75	45	15	15			

- Molecule 12 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	v1	32	Total	C	N	O	0	0	0
			160	96	32	32			
12	v2	32	Total	C	N	O	0	0	0
			160	96	32	32			
12	v3	32	Total	C	N	O	0	0	0
			160	96	32	32			
12	v4	32	Total	C	N	O	0	0	0
			160	96	32	32			
12	v5	32	Total	C	N	O	0	0	0
			160	96	32	32			
12	v6	32	Total	C	N	O	0	0	0
			160	96	32	32			

- Molecule 13 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	w1	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w2	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w3	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w4	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w5	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w6	27	Total	C	N	O	0	0	0
			135	81	27	27			

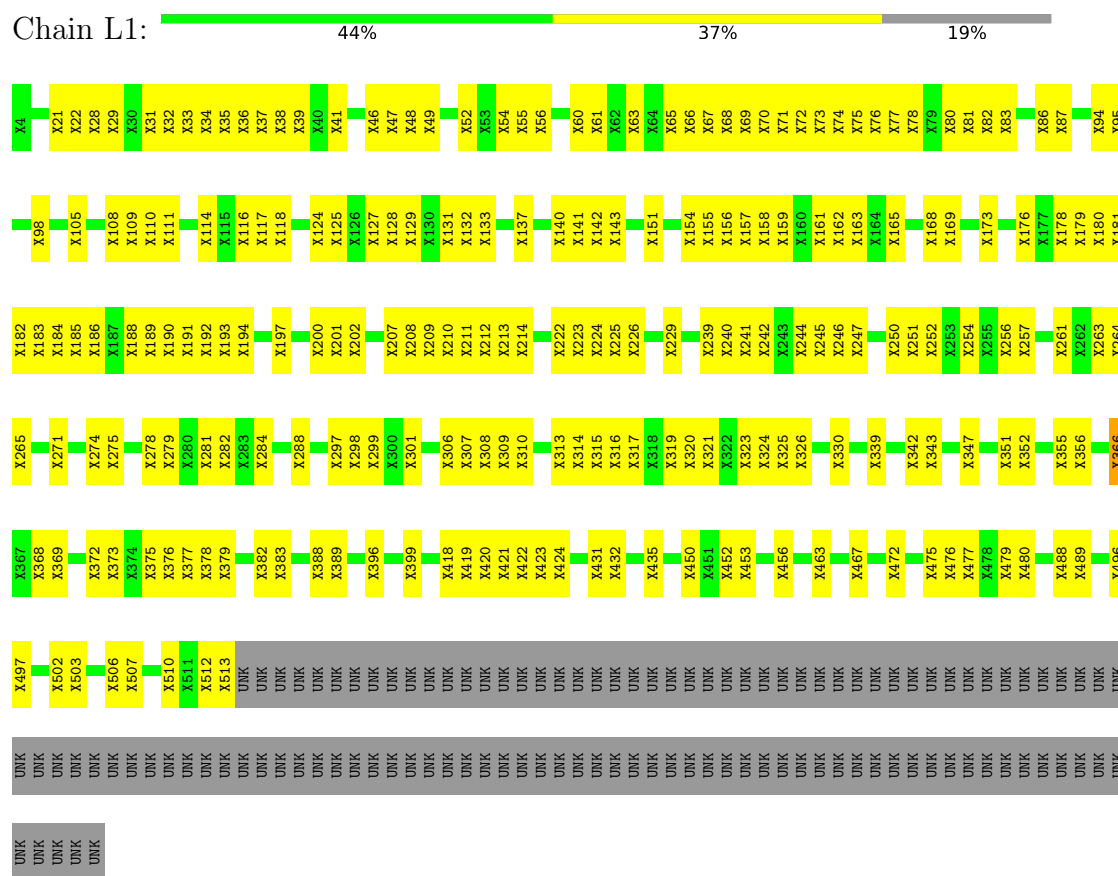
- Molecule 14 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	BA	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BB	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BC	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BD	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BE	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BF	146	Total	C	N	O	0	0	0
			730	438	146	146			

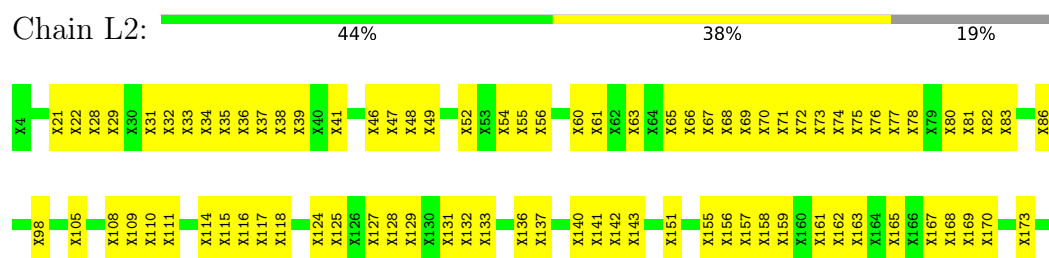
3 Residue-property plots

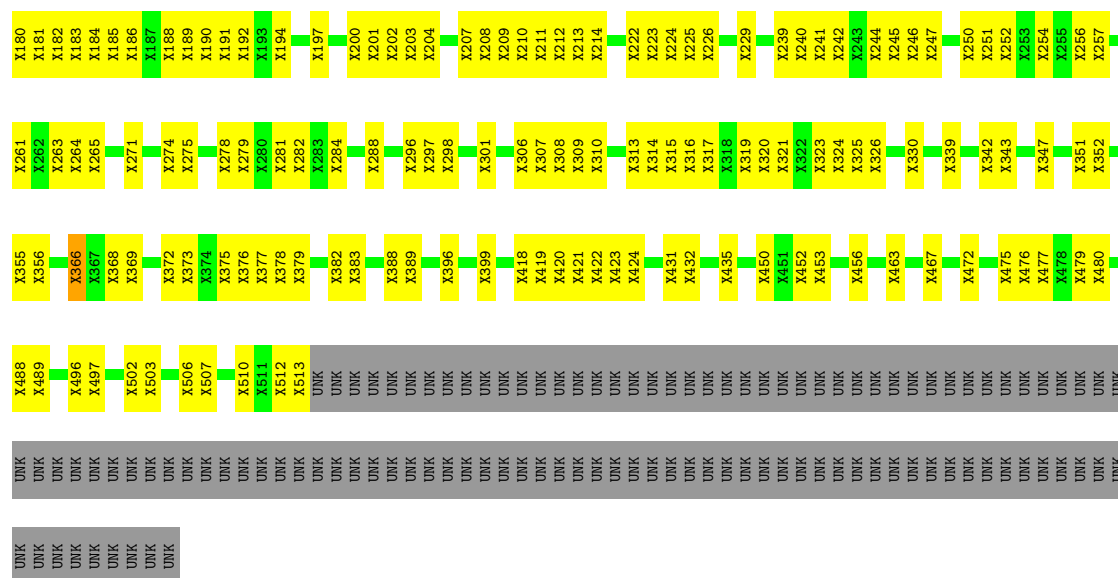
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NADH-ubiquinone oxidoreductase chain 5



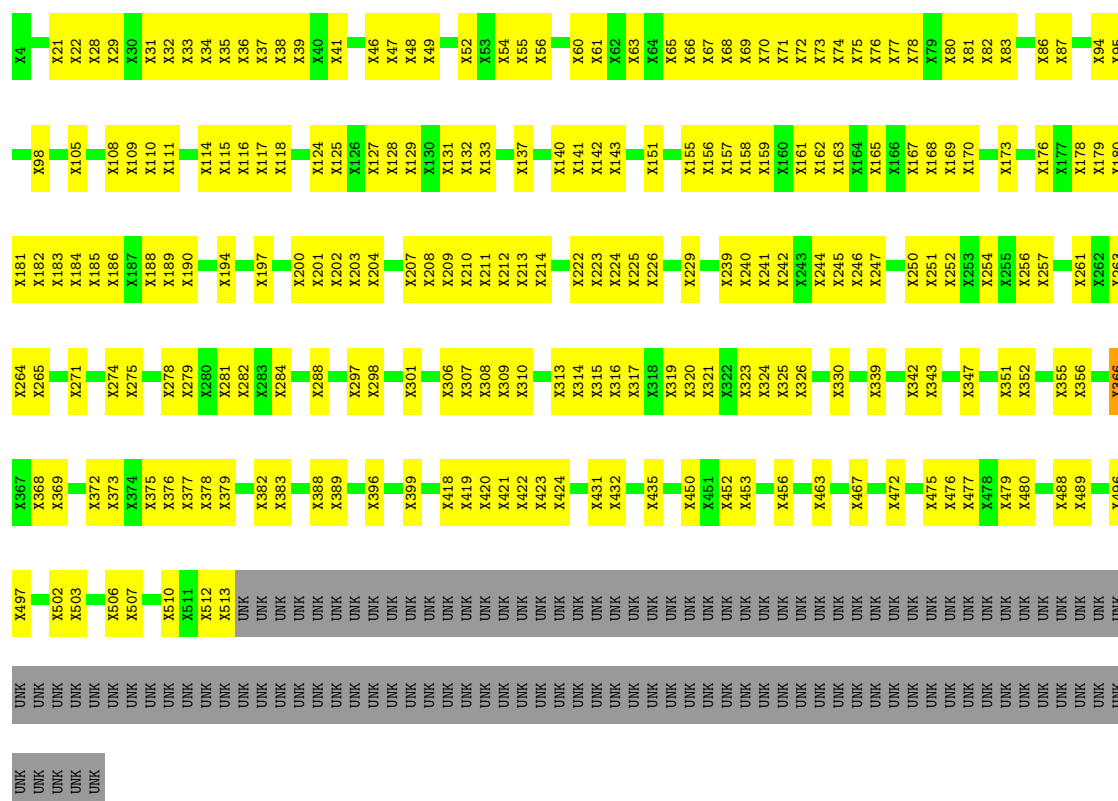
- Molecule 1: NADH-ubiquinone oxidoreductase chain 5





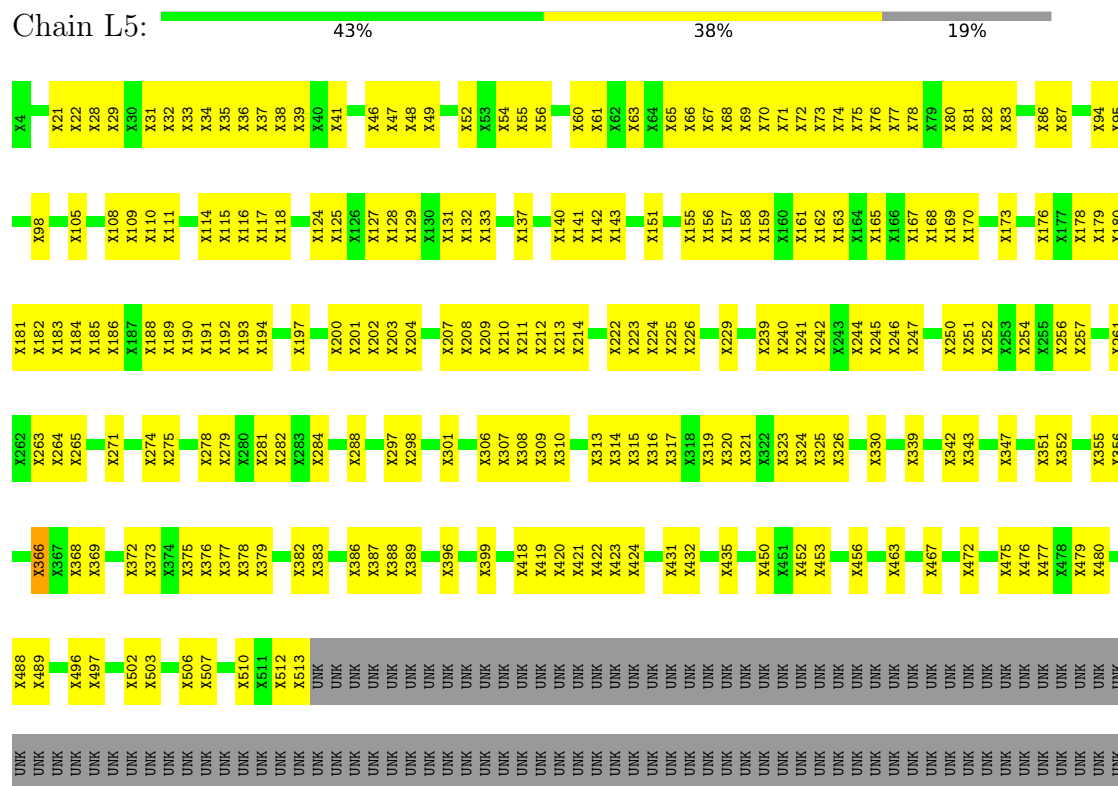
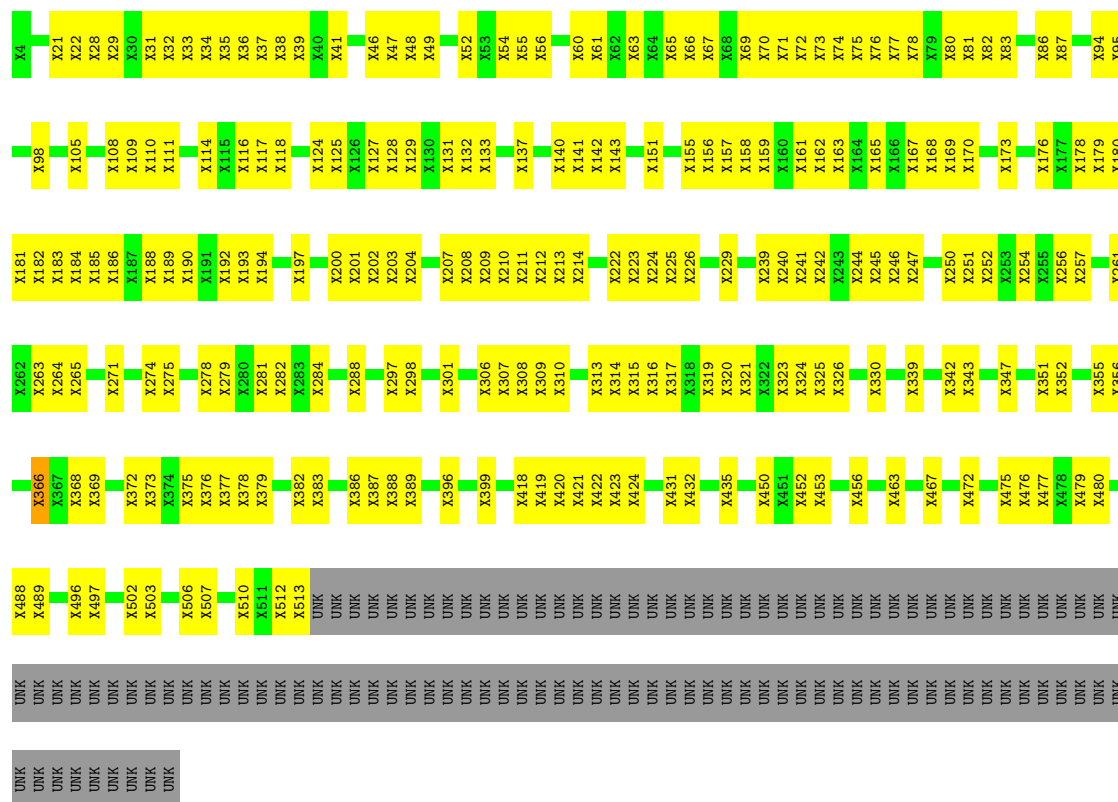
• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

Chain L3: 44% 37% 19%



• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

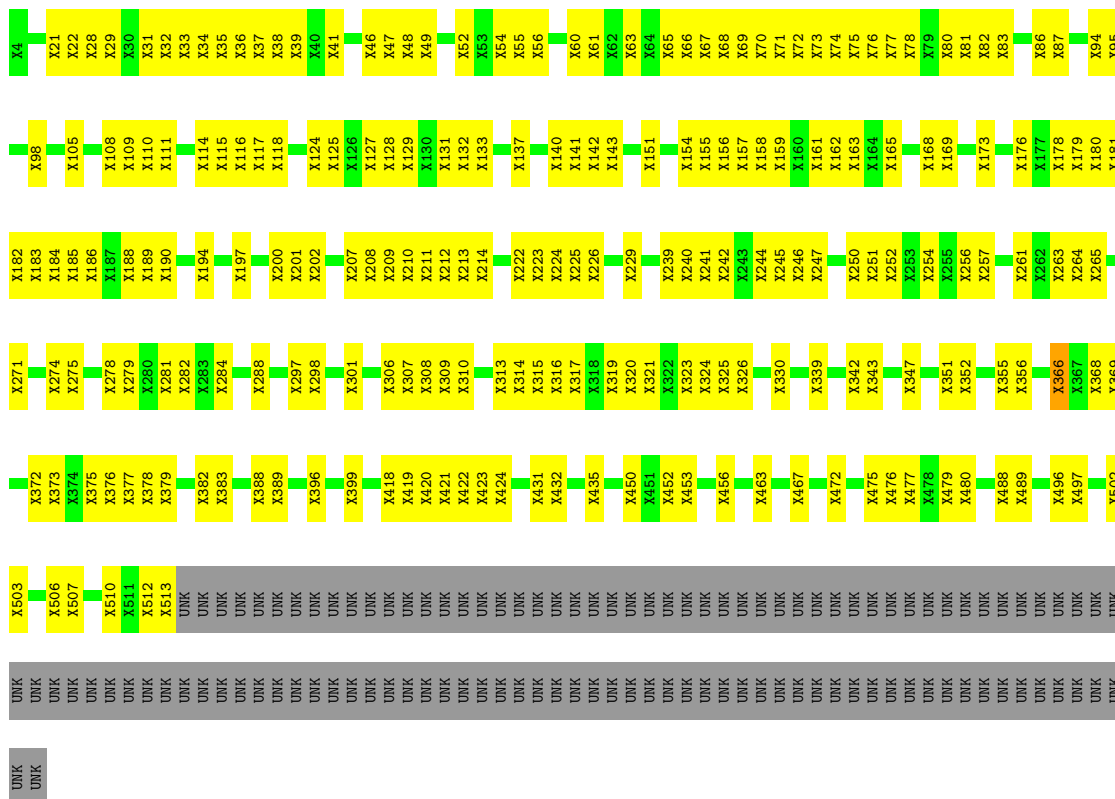
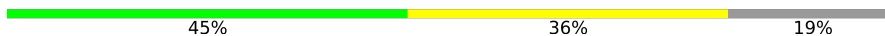
Chain L4: 44% 37% 19%



UNK UNK UNK UNK UNK UNK UNK UNK UNK

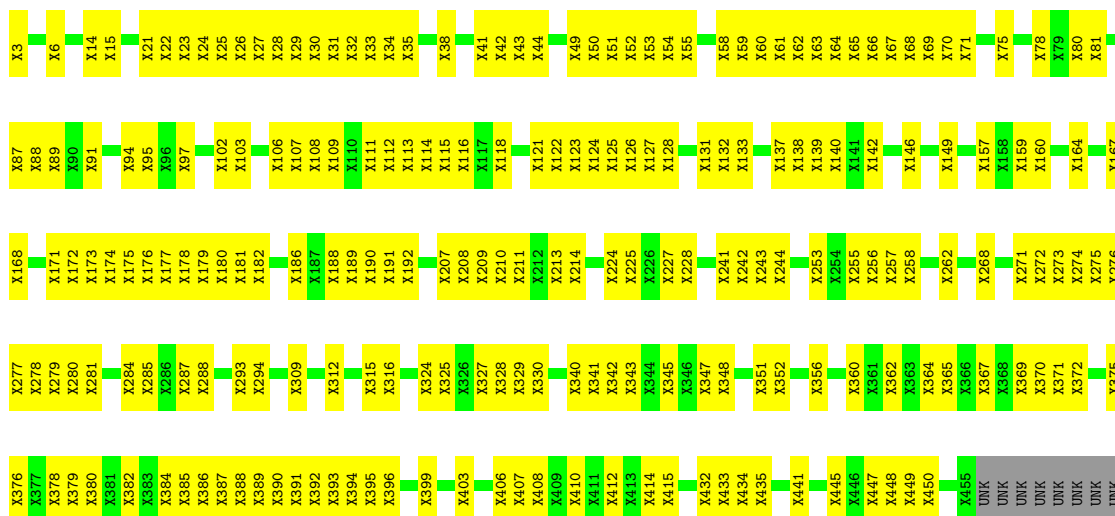
- Molecule 1: NADH-ubiquinone oxidoreductase chain 5

Chain L6:



- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

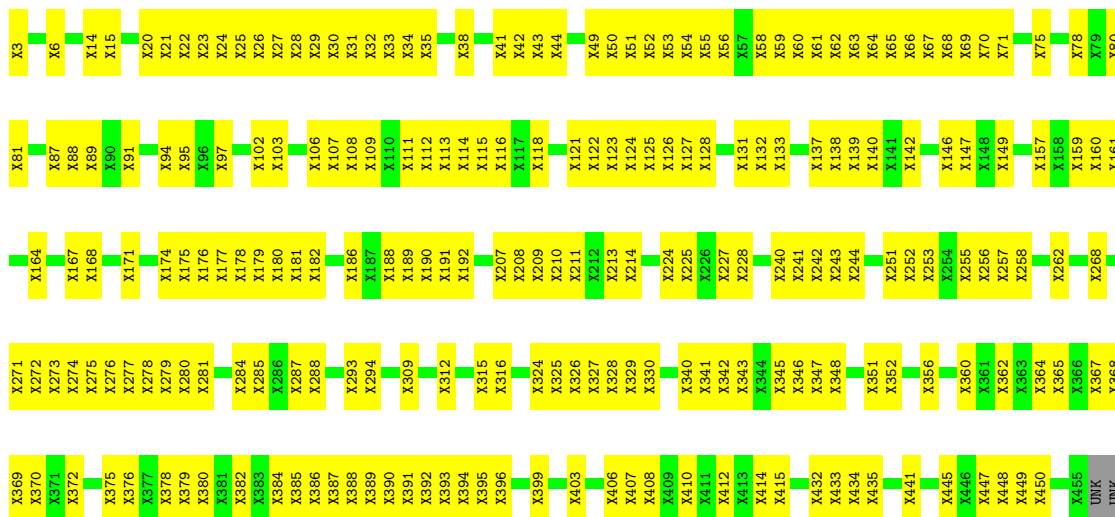
Chain M1:



UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK

• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

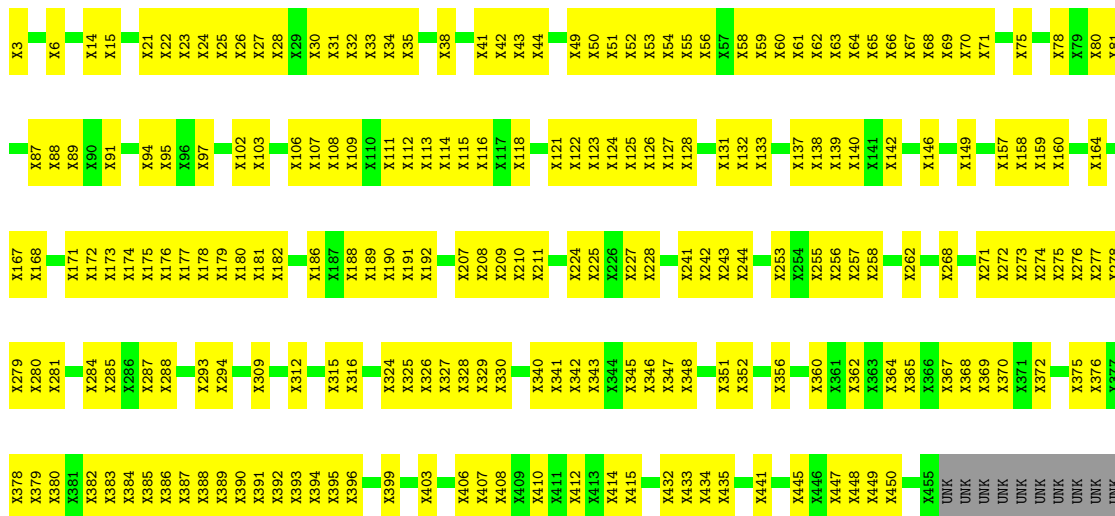
Chain M2:  47% 49% .



UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK

• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

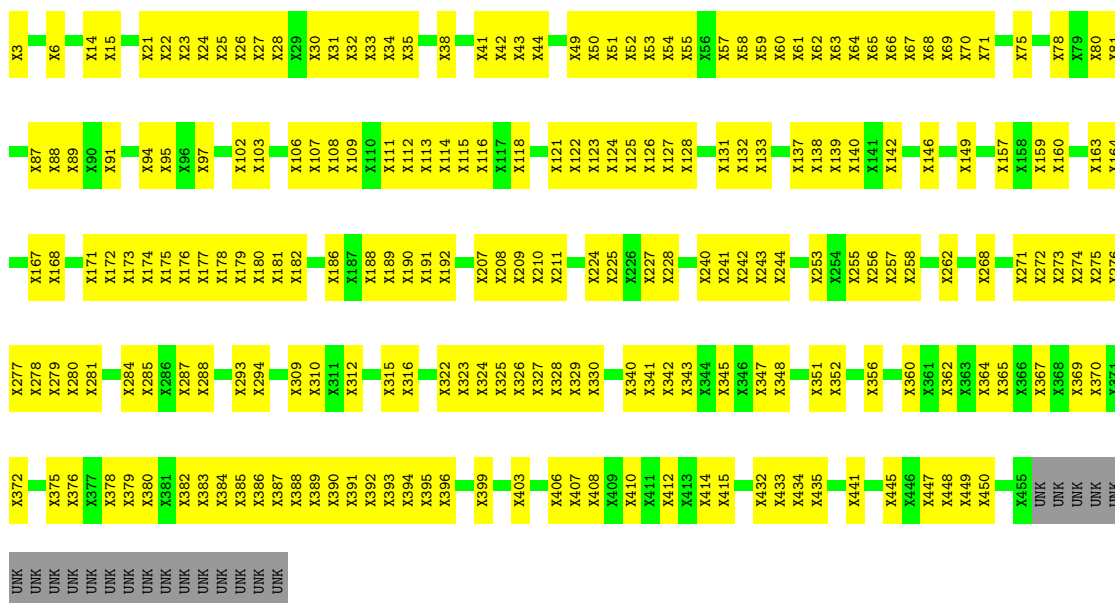
Chain M3:  48% 48% .



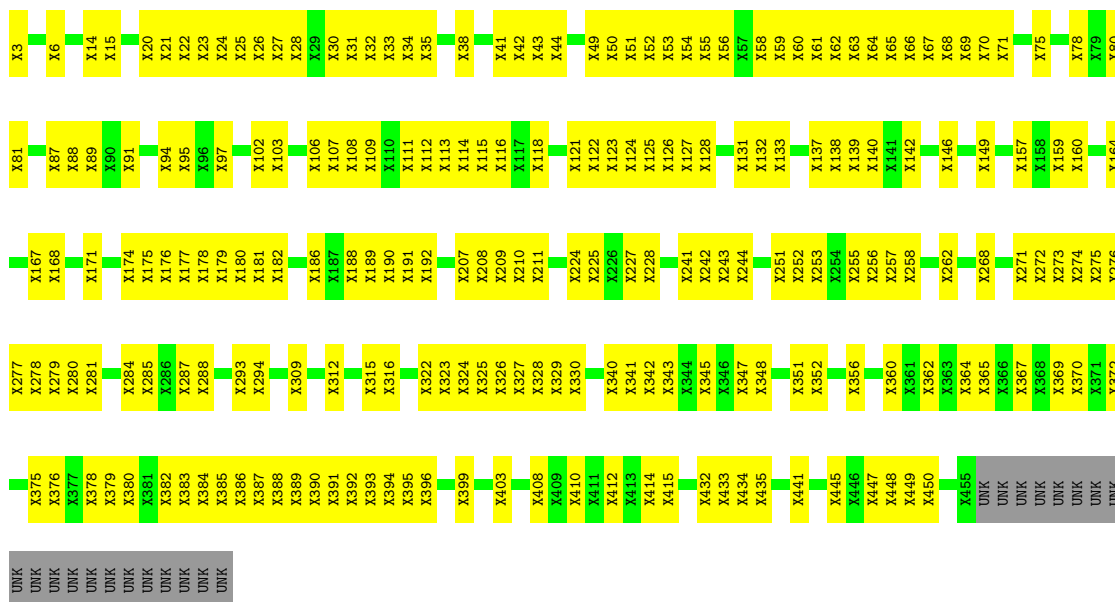
UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK

• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

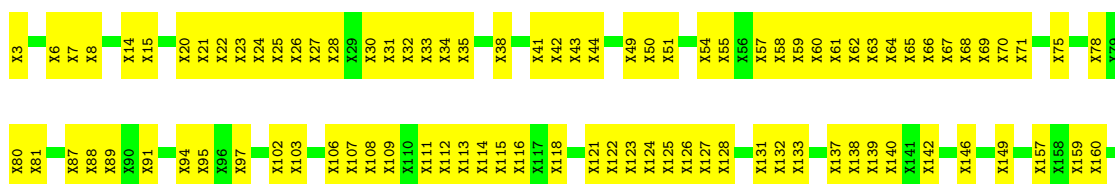
Chain M4:  47% 48% .



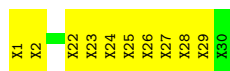
- Molecule 2: NADH-ubiquinone oxidoreductase chain 4



- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

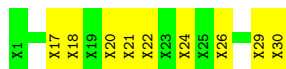







- Molecule 3: Unknown structure

Chain f3:  70% 30%



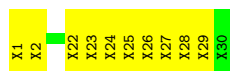
- Molecule 3: Unknown structure

Chain h3:  83% 17%



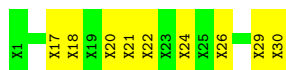
- Molecule 3: Unknown structure

Chain i3:  67% 33%




- Molecule 3: Unknown structure

Chain f4:  70% 30%



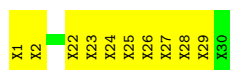
- Molecule 3: Unknown structure

Chain h4:  83% 17%



- Molecule 3: Unknown structure

Chain i4:  67% 33%

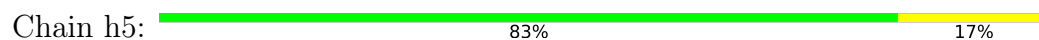


- Molecule 3: Unknown structure

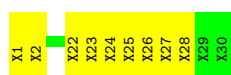
Chain f5:  70% 30%



- Molecule 3: Unknown structure



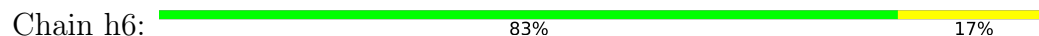
- Molecule 3: Unknown structure



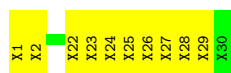
- Molecule 3: Unknown structure



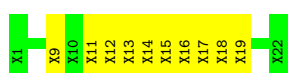
- Molecule 3: Unknown structure



- Molecule 3: Unknown structure

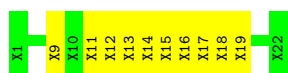


- Molecule 4: Unknown structure

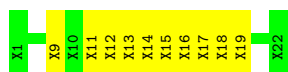


- Molecule 4: Unknown structure

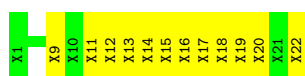




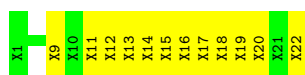
- Molecule 4: Unknown structure



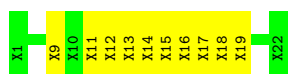
- Molecule 4: Unknown structure



- Molecule 4: Unknown structure



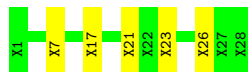
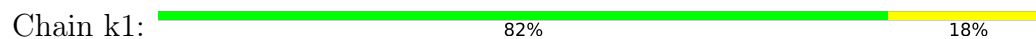
- Molecule 4: Unknown structure



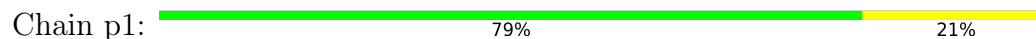
- Molecule 5: Unknown structure

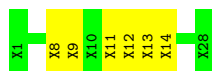


- Molecule 5: Unknown structure



- Molecule 5: Unknown structure





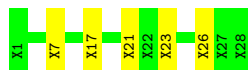
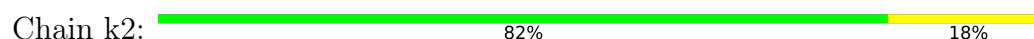
- Molecule 5: Unknown structure



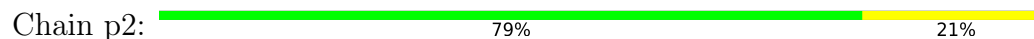
- Molecule 5: Unknown structure



- Molecule 5: Unknown structure



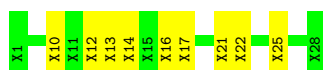
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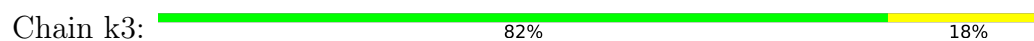
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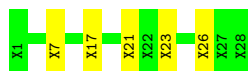


- Molecule 5: Unknown structure




- Molecule 5: Unknown structure





- Molecule 5: Unknown structure

Chain p3:  79% 21%



- Molecule 5: Unknown structure

Chain s3:  57% 43%




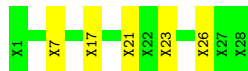
- Molecule 5: Unknown structure

Chain j4:  68% 32%




- Molecule 5: Unknown structure

Chain k4:  82% 18%



- Molecule 5: Unknown structure

Chain p4:  79% 21%



- Molecule 5: Unknown structure

Chain s4:  57% 43%

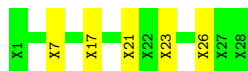
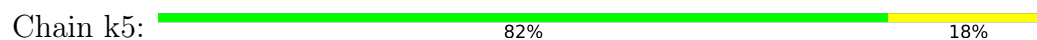


- Molecule 5: Unknown structure

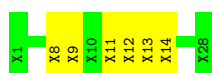
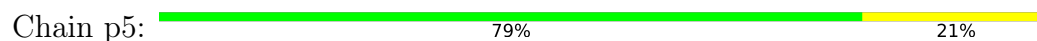
Chain j5:  68% 32%



- Molecule 5: Unknown structure



- Molecule 5: Unknown structure



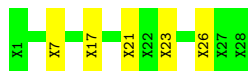
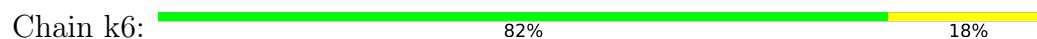
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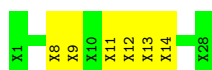
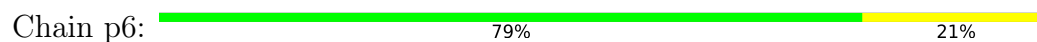
- Molecule 5: Unknown structure



- Molecule 5: Unknown structure



- Molecule 5: Unknown structure

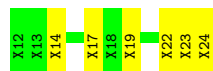


- Molecule 5: Unknown structure





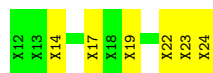
- Molecule 6: Unknown structure



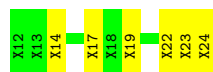
- Molecule 6: Unknown structure



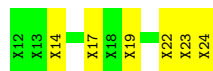
- Molecule 6: Unknown structure



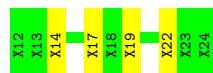
- Molecule 6: Unknown structure



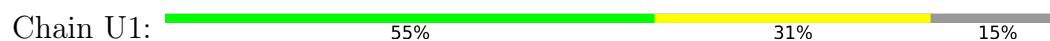
- Molecule 6: Unknown structure

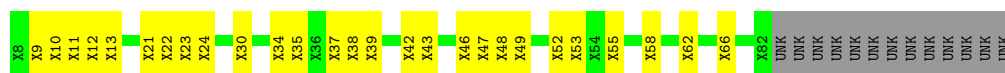


- Molecule 6: Unknown structure



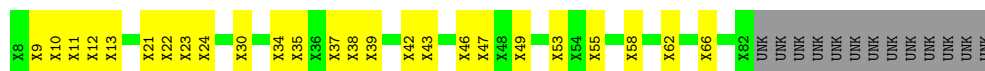
- Molecule 7: SDAP





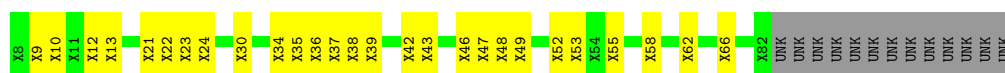
- Molecule 7: SDAP

Chain U2: 57% 28% 15%



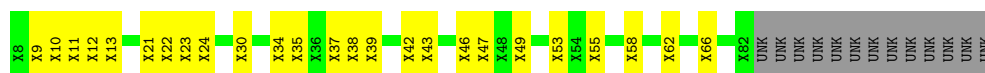
- Molecule 7: SDAP

Chain U3: 55% 31% 15%



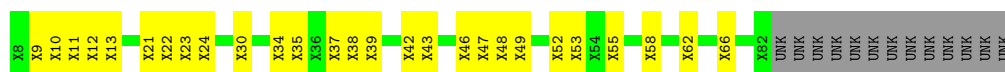
- Molecule 7: SDAP

Chain U4: 57% 28% 15%



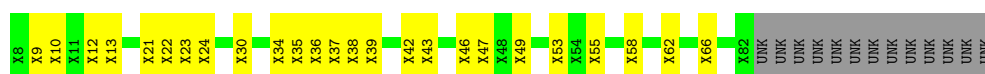
- Molecule 7: SDAP

Chain U5: 55% 31% 15%



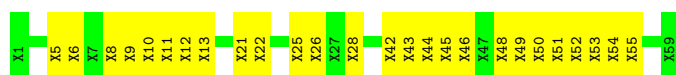
- Molecule 7: SDAP

Chain U6: 57% 28% 15%



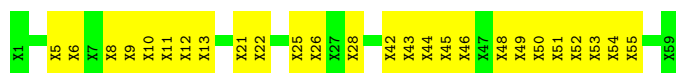
- Molecule 8: Unknown structure

Chain n1: 56% 44%

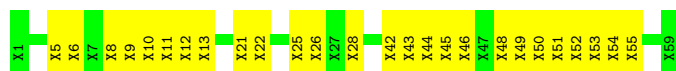


- Molecule 8: Unknown structure

Chain n2: 56% 44%



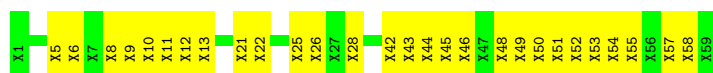
- Molecule 8: Unknown structure



- Molecule 8: Unknown structure



- Molecule 8: Unknown structure



- Molecule 8: Unknown structure



- Molecule 9: Unknown structure



There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure



There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure



There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure



There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure

Chain o5:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure

Chain o6:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: Unknown structure

Chain t1:  54% 46%



- Molecule 10: Unknown structure

Chain t2:  56% 44%



- Molecule 10: Unknown structure

Chain t3:  53% 47%




- Molecule 10: Unknown structure

Chain t4:  54% 46%




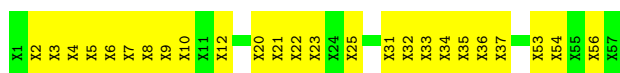
- Molecule 10: Unknown structure

Chain t5:  56% 44%



- Molecule 10: Unknown structure

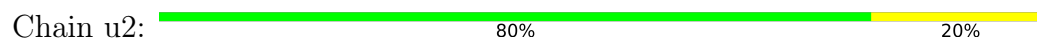
Chain t6:  56% 44%



- Molecule 11: Unknown structure



- Molecule 11: Unknown structure



- Molecule 11: Unknown structure



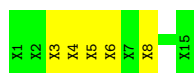
- Molecule 11: Unknown structure



- Molecule 11: Unknown structure



- Molecule 11: Unknown structure



- Molecule 12: Unknown structure





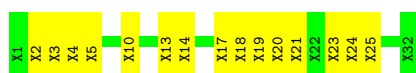
- Molecule 12: Unknown structure

Chain v2: 53% 47%



- Molecule 12: Unknown structure

Chain v3: 53% 47%



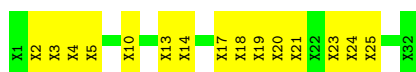
- Molecule 12: Unknown structure

Chain v4: 53% 47%



- Molecule 12: Unknown structure

Chain v5: 53% 47%



- Molecule 12: Unknown structure

Chain v6: 53% 47%



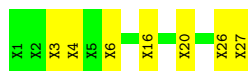
- Molecule 13: Unknown structure

Chain w1: 74% 26%

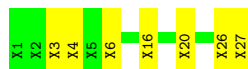
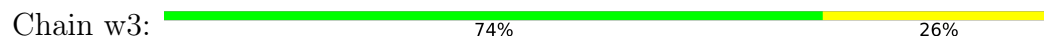


- Molecule 13: Unknown structure

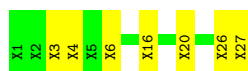
Chain w2: 74% 26%



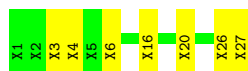
- Molecule 13: Unknown structure



- Molecule 13: Unknown structure



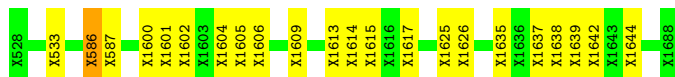
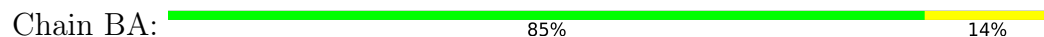
- Molecule 13: Unknown structure



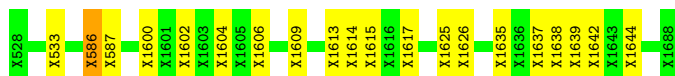
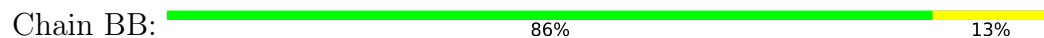
- Molecule 13: Unknown structure



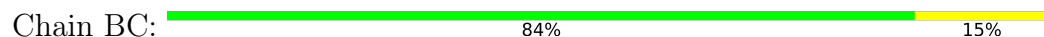
- Molecule 14: Unknown structure



- Molecule 14: Unknown structure

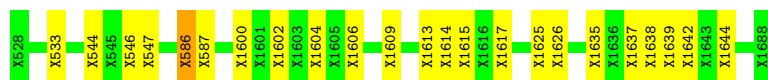
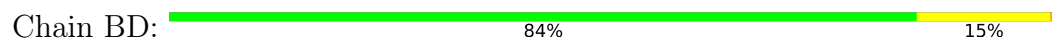


- Molecule 14: Unknown structure

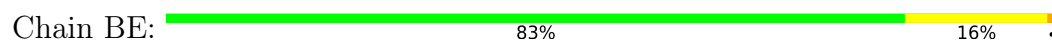




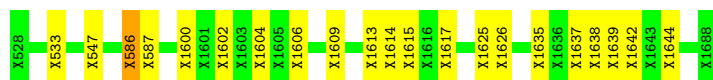
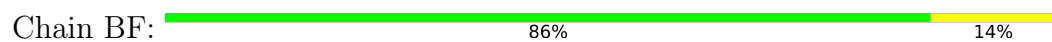
- Molecule 14: Unknown structure



- Molecule 14: Unknown structure



- Molecule 14: Unknown structure



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	244.83Å 251.41Å 412.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.69 – 6.74 41.69 – 6.74	Depositor EDS
% Data completeness (in resolution range)	97.2 (41.69-6.74) 90.7 (41.69-6.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.425 , 0.435 0.425 , 0.445	Depositor DCC
R_{free} test set	2228 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	495.7	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 731.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	48030	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L1	0	2
1	L2	0	2
1	L3	0	2
1	L4	0	2
1	L5	0	2
1	L6	0	2
14	BA	0	3
14	BB	0	3
14	BC	0	3
14	BD	0	3
14	BE	0	3
14	BF	0	3
All	All	0	30

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	BA	533	UNK	Mainchain,Peptide
14	BA	586	UNK	Mainchain
14	BB	533	UNK	Mainchain,Peptide
14	BB	586	UNK	Mainchain
14	BC	533	UNK	Mainchain,Peptide
14	BC	586	UNK	Mainchain

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Mol	Chain	Res	Type	Group
14	BD	533	UNK	Mainchain,Peptide
14	BD	586	UNK	Mainchain
14	BE	533	UNK	Mainchain,Peptide
14	BE	586	UNK	Mainchain
14	BF	533	UNK	Mainchain,Peptide
14	BF	586	UNK	Mainchain
1	L1	133	UNK	Peptide
1	L1	366	UNK	Peptide
1	L2	133	UNK	Peptide
1	L2	366	UNK	Peptide
1	L3	133	UNK	Peptide
1	L3	366	UNK	Peptide
1	L4	133	UNK	Peptide
1	L4	366	UNK	Peptide
1	L5	133	UNK	Peptide
1	L5	366	UNK	Peptide
1	L6	133	UNK	Peptide
1	L6	366	UNK	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	2465	0	517	224	0
1	L2	2465	0	517	226	0
1	L3	2465	0	517	225	0
1	L4	2465	0	517	225	0
1	L5	2465	0	517	225	0
1	L6	2465	0	517	219	0
2	M1	2195	0	455	203	0
2	M2	2195	0	455	210	0
2	M3	2195	0	455	207	0
2	M4	2195	0	455	206	0
2	M5	2195	0	455	202	0
2	M6	2195	0	455	207	0
3	f1	150	0	33	7	0
3	f2	150	0	33	7	0
3	f3	150	0	33	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	f4	150	0	33	7	0
3	f5	150	0	33	7	0
3	f6	150	0	33	7	0
3	h1	150	0	32	8	0
3	h2	150	0	32	8	0
3	h3	150	0	32	8	0
3	h4	150	0	32	7	0
3	h5	150	0	32	8	0
3	h6	150	0	32	8	0
3	i1	150	0	33	14	0
3	i2	150	0	33	14	0
3	i3	150	0	33	13	0
3	i4	150	0	33	14	0
3	i5	150	0	33	13	0
3	i6	150	0	33	14	0
4	g1	110	0	24	9	0
4	g2	110	0	24	9	0
4	g3	110	0	24	9	0
4	g4	110	0	24	10	0
4	g5	110	0	24	10	0
4	g6	110	0	24	9	0
5	j1	140	0	33	9	0
5	j2	140	0	33	9	0
5	j3	140	0	33	9	0
5	j4	140	0	33	9	0
5	j5	140	0	33	9	0
5	j6	140	0	33	9	0
5	k1	140	0	30	3	0
5	k2	140	0	30	3	0
5	k3	140	0	30	3	0
5	k4	140	0	30	3	0
5	k5	140	0	30	3	0
5	k6	140	0	30	3	0
5	p1	140	0	30	4	0
5	p2	140	0	30	4	0
5	p3	140	0	30	4	0
5	p4	140	0	30	4	0
5	p5	140	0	30	4	0
5	p6	140	0	30	4	0
5	s1	140	0	31	10	0
5	s2	140	0	31	10	0
5	s3	140	0	31	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	s4	140	0	31	11	0
5	s5	140	0	31	11	0
5	s6	140	0	31	10	0
6	l1	65	0	15	3	0
6	l2	65	0	15	3	0
6	l3	65	0	15	3	0
6	l4	65	0	15	3	0
6	l5	65	0	15	3	0
6	l6	65	0	15	2	0
7	U1	375	0	80	22	0
7	U2	375	0	80	21	0
7	U3	375	0	80	22	0
7	U4	375	0	80	21	0
7	U5	375	0	80	22	0
7	U6	375	0	80	21	0
8	n1	295	0	61	26	0
8	n2	295	0	61	26	0
8	n3	295	0	61	25	0
8	n4	295	0	61	27	0
8	n5	295	0	61	27	0
8	n6	295	0	61	24	0
9	o1	105	0	23	0	0
9	o2	105	0	23	0	0
9	o3	105	0	23	0	0
9	o4	105	0	23	0	0
9	o5	105	0	23	0	0
9	o6	105	0	23	0	0
10	t1	285	0	61	23	0
10	t2	285	0	61	22	0
10	t3	285	0	61	23	0
10	t4	285	0	61	24	0
10	t5	285	0	61	22	0
10	t6	285	0	61	22	0
11	u1	75	0	17	4	0
11	u2	75	0	17	3	0
11	u3	75	0	17	4	0
11	u4	75	0	17	4	0
11	u5	75	0	17	4	0
11	u6	75	0	17	4	0
12	v1	160	0	34	11	0
12	v2	160	0	34	11	0
12	v3	160	0	34	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	v4	160	0	34	11	0
12	v5	160	0	34	11	0
12	v6	160	0	34	11	0
13	w1	135	0	30	5	0
13	w2	135	0	29	5	0
13	w3	135	0	29	5	0
13	w4	135	0	29	5	0
13	w5	135	0	29	5	0
13	w6	135	0	29	5	0
14	BA	730	0	164	30	0
14	BB	730	0	164	29	0
14	BC	730	0	164	38	0
14	BD	730	0	164	39	0
14	BE	730	0	164	40	0
14	BF	730	0	164	39	0
All	All	48030	0	10213	3668	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 63.

All (3668) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:321:UNK:CB	1:L5:324:UNK:CB	1.91	1.48
14:BA:1609:UNK:CB	14:BA:1642:UNK:CB	1.92	1.47
1:L1:321:UNK:CB	1:L1:324:UNK:CB	1.91	1.47
1:L4:321:UNK:CB	1:L4:324:UNK:CB	1.91	1.47
14:BB:1609:UNK:CB	14:BB:1642:UNK:CB	1.92	1.46
14:BD:1609:UNK:CB	14:BD:1642:UNK:CB	1.92	1.46
14:BC:1609:UNK:CB	14:BC:1642:UNK:CB	1.92	1.46
1:L2:321:UNK:CB	1:L2:324:UNK:CB	1.91	1.45
1:L3:321:UNK:CB	1:L3:324:UNK:CB	1.91	1.45
14:BF:1609:UNK:CB	14:BF:1642:UNK:CB	1.92	1.45
1:L6:321:UNK:CB	1:L6:324:UNK:CB	1.91	1.44
14:BE:1609:UNK:CB	14:BE:1642:UNK:CB	1.92	1.44
14:BC:1614:UNK:HA	14:BC:1617:UNK:CB	1.51	1.41
14:BD:1614:UNK:HA	14:BD:1617:UNK:CB	1.51	1.40
14:BF:1614:UNK:HA	14:BF:1617:UNK:CB	1.51	1.39
14:BA:1614:UNK:HA	14:BA:1617:UNK:CB	1.51	1.39
1:L2:247:UNK:HA	1:L2:251:UNK:CB	1.52	1.39
14:BB:1614:UNK:HA	14:BB:1617:UNK:CB	1.51	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L3:247:UNK:HA	1:L3:251:UNK:CB	1.52	1.38
1:L1:247:UNK:HA	1:L1:251:UNK:CB	1.52	1.38
1:L4:247:UNK:HA	1:L4:251:UNK:CB	1.52	1.37
14:BE:1614:UNK:HA	14:BE:1617:UNK:CB	1.51	1.36
1:L5:247:UNK:HA	1:L5:251:UNK:CB	1.52	1.35
1:L6:247:UNK:HA	1:L6:251:UNK:CB	1.52	1.35
14:BC:1588:UNK:H	14:BF:547:UNK:CA	1.44	1.31
14:BC:1588:UNK:N	14:BF:547:UNK:HA	1.00	1.30
14:BC:1588:UNK:N	14:BF:547:UNK:CA	1.95	1.28
1:L4:65:UNK:CB	1:L4:67:UNK:N	1.98	1.26
1:L2:65:UNK:CB	1:L2:67:UNK:N	1.98	1.26
1:L5:65:UNK:CB	1:L5:67:UNK:N	1.98	1.26
1:L1:65:UNK:CB	1:L1:67:UNK:N	1.98	1.25
1:L6:65:UNK:CB	1:L6:67:UNK:N	1.98	1.25
1:L3:65:UNK:CB	1:L3:67:UNK:N	1.98	1.24
1:L1:161:UNK:HA	1:L1:162:UNK:C	1.65	1.24
1:L4:161:UNK:HA	1:L4:162:UNK:C	1.65	1.21
1:L3:225:UNK:HA	1:L3:229:UNK:CB	1.73	1.19
1:L3:161:UNK:HA	1:L3:162:UNK:C	1.65	1.18
1:L1:225:UNK:HA	1:L1:229:UNK:CB	1.73	1.18
1:L3:161:UNK:HA	1:L3:163:UNK:N	1.59	1.18
1:L2:161:UNK:HA	1:L2:162:UNK:C	1.65	1.18
1:L5:225:UNK:HA	1:L5:229:UNK:CB	1.73	1.18
2:M1:58:UNK:HA	2:M1:59:UNK:CB	1.71	1.17
2:M4:58:UNK:HA	2:M4:59:UNK:CB	1.71	1.17
1:L6:161:UNK:HA	1:L6:163:UNK:N	1.59	1.17
1:L2:225:UNK:HA	1:L2:229:UNK:CB	1.73	1.17
1:L4:225:UNK:HA	1:L4:229:UNK:CB	1.73	1.17
1:L1:161:UNK:HA	1:L1:163:UNK:N	1.59	1.17
1:L2:161:UNK:HA	1:L2:163:UNK:N	1.59	1.17
1:L6:225:UNK:HA	1:L6:229:UNK:CB	1.73	1.17
2:M2:58:UNK:HA	2:M2:59:UNK:CB	1.71	1.16
2:M3:58:UNK:HA	2:M3:59:UNK:CB	1.71	1.14
1:L4:161:UNK:HA	1:L4:163:UNK:N	1.59	1.14
1:L6:161:UNK:HA	1:L6:162:UNK:C	1.65	1.14
1:L5:161:UNK:HA	1:L5:163:UNK:N	1.59	1.14
2:M5:347:UNK:O	2:M5:351:UNK:N	1.81	1.14
2:M6:347:UNK:O	2:M6:351:UNK:N	1.81	1.14
2:M1:347:UNK:O	2:M1:351:UNK:N	1.81	1.13
2:M5:58:UNK:HA	2:M5:59:UNK:CB	1.71	1.13
2:M6:58:UNK:HA	2:M6:59:UNK:CB	1.71	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:161:UNK:HA	1:L5:162:UNK:C	1.65	1.12
2:M3:347:UNK:O	2:M3:351:UNK:N	1.81	1.12
2:M4:347:UNK:O	2:M4:351:UNK:N	1.81	1.12
2:M2:347:UNK:O	2:M2:351:UNK:N	1.81	1.12
1:L2:32:UNK:O	1:L2:36:UNK:N	1.87	1.08
1:L4:32:UNK:O	1:L4:36:UNK:N	1.87	1.08
1:L5:32:UNK:O	1:L5:36:UNK:N	1.87	1.08
1:L3:32:UNK:O	1:L3:36:UNK:N	1.87	1.07
7:U3:21:UNK:O	14:BC:1635:UNK:CB	2.02	1.07
3:h4:6:UNK:O	3:h4:10:UNK:CB	2.02	1.07
3:h1:6:UNK:O	3:h1:10:UNK:CB	2.02	1.07
7:U1:21:UNK:O	14:BA:1635:UNK:CB	2.02	1.07
1:L5:29:UNK:O	1:L5:33:UNK:N	1.88	1.07
1:L1:32:UNK:O	1:L1:36:UNK:N	1.87	1.07
1:L5:209:UNK:O	1:L5:212:UNK:N	1.88	1.07
3:h5:6:UNK:O	3:h5:10:UNK:CB	2.02	1.07
7:U5:21:UNK:O	14:BE:1635:UNK:CB	2.02	1.07
1:L2:209:UNK:O	1:L2:212:UNK:N	1.88	1.07
7:U2:21:UNK:O	14:BB:1635:UNK:CB	2.02	1.07
3:h3:6:UNK:O	3:h3:10:UNK:CB	2.02	1.07
1:L6:209:UNK:O	1:L6:212:UNK:N	1.88	1.06
3:h2:6:UNK:O	3:h2:10:UNK:CB	2.02	1.06
1:L3:29:UNK:O	1:L3:33:UNK:N	1.88	1.06
7:U4:21:UNK:O	14:BD:1635:UNK:CB	2.02	1.06
1:L4:29:UNK:O	1:L4:33:UNK:N	1.88	1.06
3:h6:6:UNK:O	3:h6:10:UNK:CB	2.02	1.06
1:L1:209:UNK:O	1:L1:212:UNK:N	1.88	1.06
1:L6:32:UNK:O	1:L6:36:UNK:N	1.87	1.06
7:U6:21:UNK:O	14:BF:1635:UNK:CB	2.02	1.06
1:L3:209:UNK:O	1:L3:212:UNK:N	1.88	1.05
1:L6:29:UNK:O	1:L6:33:UNK:N	1.88	1.05
1:L1:29:UNK:O	1:L1:33:UNK:N	1.88	1.05
1:L1:33:UNK:O	1:L1:37:UNK:N	1.90	1.05
1:L4:209:UNK:O	1:L4:212:UNK:N	1.88	1.05
1:L5:33:UNK:O	1:L5:37:UNK:N	1.90	1.05
1:L2:29:UNK:O	1:L2:33:UNK:N	1.88	1.05
1:L4:33:UNK:O	1:L4:37:UNK:N	1.90	1.05
1:L2:33:UNK:O	1:L2:37:UNK:N	1.90	1.04
14:BF:1614:UNK:CA	14:BF:1617:UNK:CB	2.36	1.04
1:L6:33:UNK:O	1:L6:37:UNK:N	1.90	1.04
14:BE:1614:UNK:CA	14:BE:1617:UNK:CB	2.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BA:1614:UNK:CA	14:BA:1617:UNK:CB	2.36	1.03
1:L2:181:UNK:O	1:L2:184:UNK:N	1.92	1.03
1:L3:33:UNK:O	1:L3:37:UNK:N	1.90	1.03
10:t1:2:UNK:O	10:t1:5:UNK:N	1.92	1.03
1:L4:181:UNK:O	1:L4:184:UNK:N	1.92	1.03
14:BD:1614:UNK:CA	14:BD:1617:UNK:CB	2.36	1.03
1:L5:181:UNK:O	1:L5:184:UNK:N	1.92	1.03
1:L6:181:UNK:O	1:L6:184:UNK:N	1.92	1.03
14:BB:1614:UNK:CA	14:BB:1617:UNK:CB	2.36	1.03
1:L5:28:UNK:O	1:L5:32:UNK:N	1.91	1.03
1:L4:28:UNK:O	1:L4:32:UNK:N	1.91	1.03
1:L6:28:UNK:O	1:L6:32:UNK:N	1.91	1.03
1:L3:28:UNK:O	1:L3:32:UNK:N	1.91	1.02
1:L1:181:UNK:O	1:L1:184:UNK:N	1.92	1.02
10:t6:2:UNK:O	10:t6:5:UNK:N	1.92	1.02
1:L1:28:UNK:O	1:L1:32:UNK:N	1.91	1.02
1:L2:28:UNK:O	1:L2:32:UNK:N	1.91	1.02
1:L3:181:UNK:O	1:L3:184:UNK:N	1.92	1.02
14:BC:1614:UNK:CA	14:BC:1617:UNK:CB	2.36	1.02
10:t5:2:UNK:O	10:t5:5:UNK:N	1.92	1.02
10:t2:2:UNK:O	10:t2:5:UNK:N	1.92	1.01
10:t4:2:UNK:O	10:t4:5:UNK:N	1.92	1.01
14:BD:547:UNK:O	14:BE:1590:UNK:N	1.78	1.01
10:t3:2:UNK:O	10:t3:5:UNK:N	1.92	1.01
1:L1:239:UNK:O	1:L1:240:UNK:C	2.07	1.00
1:L3:131:UNK:HA	1:L3:143:UNK:CB	1.92	1.00
1:L5:131:UNK:HA	1:L5:143:UNK:CB	1.92	1.00
1:L1:131:UNK:HA	1:L1:143:UNK:CB	1.92	1.00
1:L6:131:UNK:HA	1:L6:143:UNK:CB	1.92	1.00
1:L2:82:UNK:O	1:L2:87:UNK:N	1.95	0.99
1:L6:247:UNK:O	1:L6:252:UNK:N	1.95	0.99
1:L4:131:UNK:HA	1:L4:143:UNK:CB	1.92	0.99
1:L5:247:UNK:O	1:L5:252:UNK:N	1.95	0.99
1:L3:247:UNK:O	1:L3:252:UNK:N	1.95	0.99
1:L4:82:UNK:O	1:L4:87:UNK:N	1.95	0.99
1:L1:82:UNK:O	1:L1:87:UNK:N	1.96	0.99
1:L6:82:UNK:O	1:L6:87:UNK:N	1.96	0.99
1:L4:247:UNK:O	1:L4:252:UNK:N	1.95	0.99
1:L3:246:UNK:O	1:L3:251:UNK:N	1.96	0.99
1:L2:131:UNK:HA	1:L2:143:UNK:CB	1.92	0.98
1:L2:247:UNK:O	1:L2:252:UNK:N	1.95	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:246:UNK:O	1:L2:251:UNK:N	1.96	0.98
1:L4:246:UNK:O	1:L4:251:UNK:N	1.96	0.98
1:L1:247:UNK:O	1:L1:252:UNK:N	1.95	0.98
2:M5:388:UNK:N	2:M5:389:UNK:HA	1.79	0.98
2:M3:387:UNK:C	2:M3:389:UNK:HA	1.93	0.98
1:L5:82:UNK:O	1:L5:87:UNK:N	1.95	0.98
1:L3:82:UNK:O	1:L3:87:UNK:N	1.95	0.97
1:L3:319:UNK:O	1:L3:320:UNK:CB	2.13	0.97
2:M1:387:UNK:C	2:M1:389:UNK:HA	1.93	0.97
2:M6:387:UNK:C	2:M6:389:UNK:HA	1.93	0.97
2:M2:387:UNK:C	2:M2:389:UNK:HA	1.93	0.97
1:L6:246:UNK:O	1:L6:251:UNK:N	1.96	0.97
3:h1:9:UNK:O	3:h1:12:UNK:CB	2.13	0.97
1:L3:239:UNK:O	1:L3:240:UNK:C	2.07	0.97
1:L6:161:UNK:CA	1:L6:162:UNK:C	2.41	0.97
1:L4:189:UNK:O	1:L4:194:UNK:N	1.98	0.97
1:L4:239:UNK:O	1:L4:240:UNK:C	2.07	0.97
1:L1:246:UNK:O	1:L1:251:UNK:N	1.97	0.97
2:M4:388:UNK:N	2:M4:389:UNK:HA	1.79	0.97
3:h6:9:UNK:O	3:h6:12:UNK:CB	2.13	0.97
3:h3:9:UNK:O	3:h3:12:UNK:CB	2.13	0.96
3:h4:9:UNK:O	3:h4:12:UNK:CB	2.13	0.96
1:L6:239:UNK:O	1:L6:240:UNK:C	2.07	0.96
1:L3:189:UNK:O	1:L3:194:UNK:N	1.98	0.96
2:M6:58:UNK:CA	2:M6:59:UNK:CB	2.42	0.96
1:L2:189:UNK:O	1:L2:194:UNK:N	1.98	0.96
2:M5:387:UNK:C	2:M5:389:UNK:HA	1.93	0.96
2:M6:388:UNK:N	2:M6:389:UNK:HA	1.79	0.96
3:h5:9:UNK:O	3:h5:12:UNK:CB	2.13	0.96
2:M4:387:UNK:C	2:M4:389:UNK:HA	1.93	0.96
1:L5:246:UNK:O	1:L5:251:UNK:N	1.96	0.96
1:L6:189:UNK:O	1:L6:194:UNK:N	1.98	0.96
1:L2:239:UNK:O	1:L2:240:UNK:C	2.07	0.96
2:M5:58:UNK:CA	2:M5:59:UNK:CB	2.42	0.96
1:L1:189:UNK:O	1:L1:194:UNK:N	1.98	0.96
3:h2:9:UNK:O	3:h2:12:UNK:CB	2.13	0.95
1:L5:189:UNK:O	1:L5:194:UNK:N	1.98	0.95
1:L5:239:UNK:O	1:L5:240:UNK:C	2.07	0.95
2:M2:388:UNK:N	2:M2:389:UNK:HA	1.79	0.95
1:L1:319:UNK:O	1:L1:320:UNK:CB	2.13	0.95
5:s1:26:UNK:O	5:s1:28:UNK:O	1.84	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s2:26:UNK:O	5:s2:28:UNK:O	1.84	0.95
14:BD:547:UNK:O	14:BE:1591:UNK:N	1.99	0.95
5:s6:26:UNK:O	5:s6:28:UNK:O	1.84	0.95
2:M1:388:UNK:N	2:M1:389:UNK:HA	1.79	0.95
1:L2:319:UNK:O	1:L2:320:UNK:CB	2.12	0.95
1:L3:161:UNK:CA	1:L3:162:UNK:C	2.41	0.95
1:L5:319:UNK:O	1:L5:320:UNK:CB	2.13	0.94
5:s5:26:UNK:O	5:s5:28:UNK:O	1.84	0.94
5:s4:26:UNK:O	5:s4:28:UNK:O	1.84	0.94
5:s3:26:UNK:O	5:s3:28:UNK:O	1.84	0.94
1:L2:83:UNK:HA	1:L2:87:UNK:CB	1.98	0.94
2:M3:51:UNK:CB	2:M3:58:UNK:CB	2.46	0.94
2:M3:58:UNK:CA	2:M3:59:UNK:CB	2.42	0.94
1:L1:83:UNK:HA	1:L1:87:UNK:CB	1.98	0.94
2:M3:388:UNK:N	2:M3:389:UNK:HA	1.79	0.94
14:BC:1614:UNK:O	14:BC:1617:UNK:N	2.01	0.94
1:L6:210:UNK:O	1:L6:214:UNK:N	2.01	0.94
2:M4:51:UNK:CB	2:M4:58:UNK:CB	2.46	0.94
2:M6:51:UNK:CB	2:M6:58:UNK:CB	2.46	0.94
1:L1:161:UNK:CA	1:L1:162:UNK:C	2.41	0.94
1:L5:83:UNK:HA	1:L5:87:UNK:CB	1.98	0.94
8:n5:43:UNK:O	8:n5:46:UNK:N	2.01	0.94
1:L6:83:UNK:HA	1:L6:87:UNK:CB	1.98	0.93
8:n1:43:UNK:O	8:n1:46:UNK:N	2.01	0.93
8:n3:43:UNK:O	8:n3:46:UNK:N	2.01	0.93
2:M6:103:UNK:O	2:M6:107:UNK:N	2.02	0.93
2:M4:103:UNK:O	2:M4:107:UNK:N	2.02	0.93
2:M5:103:UNK:O	2:M5:107:UNK:N	2.02	0.93
2:M1:103:UNK:O	2:M1:107:UNK:N	2.02	0.93
2:M2:51:UNK:CB	2:M2:58:UNK:CB	2.46	0.93
1:L3:210:UNK:O	1:L3:214:UNK:N	2.01	0.93
1:L4:319:UNK:O	1:L4:320:UNK:CB	2.13	0.93
8:n4:43:UNK:O	8:n4:46:UNK:N	2.01	0.93
2:M3:103:UNK:O	2:M3:107:UNK:N	2.02	0.93
1:L4:83:UNK:HA	1:L4:87:UNK:CB	1.98	0.93
1:L3:83:UNK:HA	1:L3:87:UNK:CB	1.98	0.93
1:L4:210:UNK:O	1:L4:214:UNK:N	2.01	0.93
1:L5:55:UNK:N	1:L5:56:UNK:O	2.02	0.93
1:L1:210:UNK:O	1:L1:214:UNK:N	2.01	0.93
2:M1:51:UNK:CB	2:M1:58:UNK:CB	2.46	0.93
2:M2:58:UNK:CA	2:M2:59:UNK:CB	2.42	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BD:1614:UNK:O	14:BD:1617:UNK:N	2.01	0.93
14:BB:1614:UNK:O	14:BB:1617:UNK:N	2.01	0.92
1:L5:210:UNK:O	1:L5:214:UNK:N	2.01	0.92
1:L2:55:UNK:N	1:L2:56:UNK:O	2.02	0.92
1:L4:55:UNK:N	1:L4:56:UNK:O	2.02	0.92
2:M5:51:UNK:CB	2:M5:58:UNK:CB	2.46	0.92
1:L1:55:UNK:N	1:L1:56:UNK:O	2.02	0.92
1:L1:321:UNK:O	1:L1:324:UNK:CB	2.18	0.92
1:L2:210:UNK:O	1:L2:214:UNK:N	2.01	0.92
2:M2:103:UNK:O	2:M2:107:UNK:N	2.02	0.92
1:L3:55:UNK:N	1:L3:56:UNK:O	2.02	0.92
1:L6:319:UNK:O	1:L6:320:UNK:CB	2.13	0.92
1:L5:247:UNK:CA	1:L5:251:UNK:CB	2.47	0.92
1:L6:321:UNK:O	1:L6:324:UNK:CB	2.18	0.92
1:L2:321:UNK:O	1:L2:324:UNK:CB	2.18	0.92
8:n2:43:UNK:O	8:n2:46:UNK:N	2.01	0.92
2:M1:58:UNK:CA	2:M1:59:UNK:CB	2.42	0.92
2:M5:189:UNK:N	2:M5:191:UNK:O	2.03	0.92
8:n6:43:UNK:O	8:n6:46:UNK:N	2.01	0.91
1:L3:247:UNK:CA	1:L3:251:UNK:CB	2.47	0.91
1:L3:321:UNK:O	1:L3:324:UNK:CB	2.18	0.91
1:L4:321:UNK:O	1:L4:324:UNK:CB	2.18	0.91
2:M1:189:UNK:N	2:M1:191:UNK:O	2.03	0.91
2:M4:189:UNK:N	2:M4:191:UNK:O	2.03	0.91
1:L6:55:UNK:N	1:L6:56:UNK:O	2.02	0.91
2:M3:189:UNK:N	2:M3:191:UNK:O	2.03	0.91
1:L5:321:UNK:O	1:L5:324:UNK:CB	2.18	0.91
14:BE:1614:UNK:O	14:BE:1617:UNK:N	2.01	0.91
14:BA:1614:UNK:O	14:BA:1617:UNK:N	2.01	0.91
2:M2:189:UNK:N	2:M2:191:UNK:O	2.03	0.91
2:M6:189:UNK:N	2:M6:191:UNK:O	2.03	0.90
1:L4:161:UNK:CA	1:L4:162:UNK:C	2.41	0.90
14:BD:547:UNK:CB	14:BE:1590:UNK:N	2.34	0.90
8:n1:5:UNK:O	8:n1:8:UNK:N	2.05	0.90
1:L5:263:UNK:O	1:L5:265:UNK:N	2.05	0.90
1:L4:263:UNK:O	1:L4:265:UNK:N	2.05	0.90
14:BF:1614:UNK:O	14:BF:1617:UNK:N	2.01	0.90
2:M4:58:UNK:CA	2:M4:59:UNK:CB	2.42	0.90
2:M1:68:UNK:O	2:M1:69:UNK:C	2.19	0.90
2:M1:347:UNK:O	2:M1:351:UNK:CB	2.21	0.89
1:L3:263:UNK:O	1:L3:265:UNK:N	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:247:UNK:CA	1:L1:251:UNK:CB	2.47	0.89
8:n6:5:UNK:O	8:n6:8:UNK:N	2.05	0.89
2:M5:347:UNK:O	2:M5:351:UNK:CB	2.21	0.89
1:L6:263:UNK:O	1:L6:265:UNK:N	2.05	0.89
1:L1:263:UNK:O	1:L1:265:UNK:N	2.05	0.89
1:L3:151:UNK:O	1:L3:155:UNK:CB	2.21	0.89
1:L4:151:UNK:O	1:L4:155:UNK:CB	2.21	0.89
1:L5:151:UNK:O	1:L5:155:UNK:CB	2.21	0.89
2:M6:348:UNK:HA	2:M6:351:UNK:CB	2.03	0.89
1:L2:263:UNK:O	1:L2:265:UNK:N	2.05	0.89
2:M2:68:UNK:O	2:M2:69:UNK:C	2.19	0.89
7:U5:23:UNK:CB	7:U5:24:UNK:HA	2.03	0.89
2:M1:348:UNK:HA	2:M1:351:UNK:CB	2.03	0.89
8:n3:5:UNK:O	8:n3:8:UNK:N	2.05	0.89
8:n4:5:UNK:O	8:n4:8:UNK:N	2.05	0.89
1:L5:161:UNK:CA	1:L5:162:UNK:C	2.41	0.89
2:M5:348:UNK:HA	2:M5:351:UNK:CB	2.03	0.89
7:U1:23:UNK:CB	7:U1:24:UNK:HA	2.03	0.89
8:n2:5:UNK:O	8:n2:8:UNK:N	2.05	0.89
2:M4:348:UNK:HA	2:M4:351:UNK:CB	2.03	0.89
7:U3:23:UNK:CB	7:U3:24:UNK:HA	2.03	0.89
5:j4:21:UNK:O	5:j4:22:UNK:O	1.91	0.89
14:BA:1637:UNK:HA	14:BA:1638:UNK:C	2.03	0.88
1:L2:29:UNK:HA	1:L2:32:UNK:CB	2.03	0.88
2:M3:347:UNK:O	2:M3:351:UNK:CB	2.21	0.88
8:n5:5:UNK:O	8:n5:8:UNK:N	2.05	0.88
1:L6:151:UNK:O	1:L6:155:UNK:CB	2.21	0.88
1:L3:29:UNK:HA	1:L3:32:UNK:CB	2.03	0.88
2:M3:348:UNK:HA	2:M3:351:UNK:CB	2.03	0.88
7:U4:23:UNK:CB	7:U4:24:UNK:HA	2.03	0.88
2:M3:68:UNK:O	2:M3:69:UNK:C	2.19	0.88
14:BC:1588:UNK:H2	14:BF:547:UNK:HA	1.33	0.88
2:M4:347:UNK:O	2:M4:351:UNK:CB	2.21	0.88
5:j5:21:UNK:O	5:j5:22:UNK:O	1.91	0.88
1:L6:29:UNK:HA	1:L6:32:UNK:CB	2.03	0.88
14:BE:1637:UNK:HA	14:BE:1638:UNK:C	2.03	0.88
2:M2:347:UNK:O	2:M2:351:UNK:CB	2.21	0.88
2:M2:348:UNK:HA	2:M2:351:UNK:CB	2.03	0.88
14:BB:1637:UNK:HA	14:BB:1638:UNK:C	2.03	0.88
1:L1:29:UNK:HA	1:L1:32:UNK:CB	2.03	0.88
1:L4:29:UNK:HA	1:L4:32:UNK:CB	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BF:1637:UNK:HA	14:BF:1638:UNK:C	2.03	0.88
1:L1:151:UNK:O	1:L1:155:UNK:CB	2.21	0.88
2:M6:347:UNK:O	2:M6:351:UNK:CB	2.21	0.88
1:L5:29:UNK:HA	1:L5:32:UNK:CB	2.03	0.88
1:L6:247:UNK:CA	1:L6:251:UNK:CB	2.47	0.88
2:M6:176:UNK:N	2:M6:177:UNK:HA	1.89	0.88
1:L2:151:UNK:O	1:L2:155:UNK:CB	2.21	0.88
2:M3:49:UNK:HA	2:M3:50:UNK:CB	2.04	0.88
1:L2:161:UNK:CA	1:L2:162:UNK:C	2.41	0.87
14:BD:1637:UNK:HA	14:BD:1638:UNK:C	2.03	0.87
2:M4:49:UNK:HA	2:M4:50:UNK:CB	2.04	0.87
5:j2:21:UNK:O	5:j2:22:UNK:O	1.91	0.87
7:U6:23:UNK:CB	7:U6:24:UNK:HA	2.03	0.87
14:BC:1637:UNK:HA	14:BC:1638:UNK:C	2.03	0.87
1:L4:67:UNK:CB	1:L4:76:UNK:HA	2.05	0.87
2:M6:68:UNK:O	2:M6:69:UNK:C	2.19	0.87
5:j1:21:UNK:O	5:j1:22:UNK:O	1.91	0.87
1:L2:67:UNK:CB	1:L2:76:UNK:HA	2.05	0.87
7:U2:23:UNK:CB	7:U2:24:UNK:HA	2.03	0.87
1:L3:67:UNK:CB	1:L3:76:UNK:HA	2.05	0.87
1:L4:247:UNK:CA	1:L4:251:UNK:CB	2.47	0.87
1:L6:67:UNK:CB	1:L6:76:UNK:HA	2.05	0.87
2:M6:49:UNK:HA	2:M6:50:UNK:CB	2.04	0.87
5:j3:21:UNK:O	5:j3:22:UNK:O	1.91	0.87
14:BD:1638:UNK:HA	14:BD:1642:UNK:CB	2.05	0.87
5:j6:21:UNK:O	5:j6:22:UNK:O	1.91	0.87
1:L1:321:UNK:O	1:L1:324:UNK:N	2.08	0.86
14:BB:1638:UNK:HA	14:BB:1642:UNK:CB	2.05	0.86
1:L1:67:UNK:CB	1:L1:76:UNK:HA	2.05	0.86
3:f3:20:UNK:O	3:f3:24:UNK:N	2.08	0.86
2:M1:281:UNK:O	2:M1:284:UNK:CB	2.24	0.86
2:M2:176:UNK:N	2:M2:177:UNK:HA	1.89	0.86
1:L2:247:UNK:CA	1:L2:251:UNK:CB	2.47	0.86
1:L5:67:UNK:CB	1:L5:76:UNK:HA	2.05	0.86
2:M5:68:UNK:O	2:M5:69:UNK:C	2.19	0.86
14:BE:1638:UNK:HA	14:BE:1642:UNK:CB	2.05	0.86
3:f6:20:UNK:O	3:f6:24:UNK:N	2.08	0.86
2:M1:146:UNK:O	2:M1:149:UNK:N	2.09	0.86
2:M2:49:UNK:HA	2:M2:50:UNK:CB	2.04	0.86
2:M4:281:UNK:O	2:M4:284:UNK:CB	2.24	0.86
2:M5:176:UNK:N	2:M5:177:UNK:HA	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M1:49:UNK:HA	2:M1:50:UNK:CB	2.05	0.86
1:L5:321:UNK:O	1:L5:324:UNK:N	2.08	0.86
2:M6:281:UNK:O	2:M6:284:UNK:CB	2.24	0.86
2:M3:146:UNK:O	2:M3:149:UNK:N	2.09	0.86
2:M5:49:UNK:HA	2:M5:50:UNK:CB	2.05	0.86
2:M5:281:UNK:O	2:M5:284:UNK:CB	2.24	0.86
1:L6:316:UNK:O	1:L6:319:UNK:N	2.09	0.86
1:L6:321:UNK:O	1:L6:324:UNK:N	2.08	0.86
14:BF:1638:UNK:HA	14:BF:1642:UNK:CB	2.05	0.86
1:L1:316:UNK:O	1:L1:319:UNK:N	2.09	0.86
2:M3:281:UNK:O	2:M3:284:UNK:CB	2.24	0.86
3:f2:20:UNK:O	3:f2:24:UNK:N	2.08	0.85
1:L3:321:UNK:O	1:L3:324:UNK:N	2.08	0.85
1:L4:321:UNK:O	1:L4:324:UNK:N	2.08	0.85
2:M4:176:UNK:N	2:M4:177:UNK:HA	1.89	0.85
2:M6:146:UNK:O	2:M6:149:UNK:N	2.09	0.85
1:L5:316:UNK:O	1:L5:319:UNK:N	2.09	0.85
1:L2:297:UNK:HA	1:L2:356:UNK:N	1.92	0.85
14:BC:1638:UNK:HA	14:BC:1642:UNK:CB	2.05	0.85
3:f4:20:UNK:O	3:f4:24:UNK:N	2.08	0.85
1:L5:297:UNK:HA	1:L5:356:UNK:N	1.91	0.85
2:M1:176:UNK:N	2:M1:177:UNK:HA	1.89	0.85
1:L4:297:UNK:HA	1:L4:356:UNK:N	1.91	0.85
1:L1:297:UNK:HA	1:L1:356:UNK:N	1.91	0.85
2:M2:146:UNK:O	2:M2:149:UNK:N	2.09	0.85
1:L3:316:UNK:O	1:L3:319:UNK:N	2.09	0.85
1:L4:316:UNK:O	1:L4:319:UNK:N	2.09	0.85
2:M4:146:UNK:O	2:M4:149:UNK:N	2.09	0.85
3:f5:20:UNK:O	3:f5:24:UNK:N	2.08	0.85
14:BA:1638:UNK:HA	14:BA:1642:UNK:CB	2.05	0.85
2:M5:146:UNK:O	2:M5:149:UNK:N	2.09	0.85
1:L2:321:UNK:O	1:L2:324:UNK:N	2.08	0.85
3:f6:26:UNK:O	3:f6:29:UNK:CB	2.25	0.85
2:M4:68:UNK:O	2:M4:69:UNK:C	2.19	0.85
1:L5:46:UNK:O	1:L5:49:UNK:CB	2.25	0.85
1:L6:46:UNK:O	1:L6:49:UNK:CB	2.25	0.85
3:f3:26:UNK:O	3:f3:29:UNK:CB	2.25	0.85
3:f4:26:UNK:O	3:f4:29:UNK:CB	2.25	0.85
2:M2:281:UNK:O	2:M2:284:UNK:CB	2.24	0.84
10:t6:33:UNK:O	10:t6:36:UNK:CB	2.25	0.84
3:f1:20:UNK:O	3:f1:24:UNK:N	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:316:UNK:O	1:L2:319:UNK:N	2.09	0.84
5:j4:12:UNK:HA	5:k4:7:UNK:CB	2.07	0.84
3:f1:26:UNK:O	3:f1:29:UNK:CB	2.25	0.84
3:f2:26:UNK:O	3:f2:29:UNK:CB	2.25	0.84
2:M3:176:UNK:N	2:M3:177:UNK:HA	1.89	0.84
1:L5:288:UNK:CB	1:L5:308:UNK:CB	2.56	0.84
10:t5:33:UNK:O	10:t5:36:UNK:CB	2.26	0.84
14:BF:1602:UNK:C	14:BF:1606:UNK:N	2.30	0.84
10:t2:33:UNK:O	10:t2:36:UNK:CB	2.25	0.84
1:L3:297:UNK:HA	1:L3:356:UNK:N	1.92	0.84
10:t3:33:UNK:O	10:t3:36:UNK:CB	2.25	0.84
1:L4:34:UNK:O	1:L4:38:UNK:N	2.11	0.84
1:L4:288:UNK:CB	1:L4:308:UNK:CB	2.56	0.84
1:L6:34:UNK:O	1:L6:38:UNK:N	2.10	0.84
1:L4:46:UNK:O	1:L4:49:UNK:CB	2.25	0.84
1:L1:34:UNK:O	1:L1:38:UNK:N	2.10	0.84
5:j1:12:UNK:HA	5:k1:7:UNK:CB	2.07	0.84
5:j3:12:UNK:HA	5:k3:7:UNK:CB	2.08	0.84
1:L5:34:UNK:O	1:L5:38:UNK:N	2.10	0.84
5:j6:12:UNK:HA	5:k6:7:UNK:CB	2.07	0.84
10:t1:33:UNK:O	10:t1:36:UNK:CB	2.25	0.84
10:t4:33:UNK:O	10:t4:36:UNK:CB	2.25	0.84
1:L1:46:UNK:O	1:L1:49:UNK:CB	2.25	0.84
1:L1:197:UNK:O	1:L1:201:UNK:N	2.11	0.84
10:t3:34:UNK:O	10:t3:37:UNK:N	2.11	0.84
1:L6:197:UNK:O	1:L6:201:UNK:N	2.11	0.83
1:L2:34:UNK:O	1:L2:38:UNK:N	2.10	0.83
1:L4:197:UNK:O	1:L4:201:UNK:N	2.11	0.83
10:t4:34:UNK:O	10:t4:37:UNK:N	2.11	0.83
3:f5:26:UNK:O	3:f5:29:UNK:CB	2.25	0.83
1:L3:197:UNK:O	1:L3:201:UNK:N	2.11	0.83
5:j5:12:UNK:HA	5:k5:7:UNK:CB	2.07	0.83
1:L6:297:UNK:HA	1:L6:356:UNK:N	1.92	0.83
1:L2:46:UNK:O	1:L2:49:UNK:CB	2.25	0.83
1:L3:46:UNK:O	1:L3:49:UNK:CB	2.25	0.83
1:L6:288:UNK:CB	1:L6:308:UNK:CB	2.55	0.83
1:L3:288:UNK:CB	1:L3:308:UNK:CB	2.56	0.83
5:j2:12:UNK:HA	5:k2:7:UNK:CB	2.07	0.83
1:L1:288:UNK:CB	1:L1:308:UNK:CB	2.56	0.83
1:L2:197:UNK:O	1:L2:201:UNK:N	2.11	0.83
1:L3:34:UNK:O	1:L3:38:UNK:N	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:t5:34:UNK:O	10:t5:37:UNK:N	2.11	0.83
10:t6:34:UNK:O	10:t6:37:UNK:N	2.11	0.83
1:L2:288:UNK:CB	1:L2:308:UNK:CB	2.56	0.83
1:L3:321:UNK:O	1:L3:325:UNK:N	2.12	0.83
1:L5:197:UNK:O	1:L5:201:UNK:N	2.11	0.83
10:t2:34:UNK:O	10:t2:37:UNK:N	2.11	0.83
14:BC:1602:UNK:C	14:BC:1606:UNK:N	2.30	0.82
8:n6:10:UNK:O	8:n6:13:UNK:N	2.12	0.82
2:M3:210:UNK:HA	2:M3:268:UNK:CB	2.09	0.82
8:n2:10:UNK:O	8:n2:13:UNK:N	2.12	0.82
3:i6:22:UNK:O	3:i6:25:UNK:N	2.13	0.82
3:i2:22:UNK:O	3:i2:25:UNK:N	2.13	0.82
1:L3:77:UNK:HA	1:L3:78:UNK:CB	2.10	0.82
2:M6:281:UNK:O	2:M6:285:UNK:N	2.12	0.82
1:L1:77:UNK:HA	1:L1:78:UNK:CB	2.10	0.82
10:t1:34:UNK:O	10:t1:37:UNK:N	2.11	0.82
1:L4:77:UNK:HA	1:L4:78:UNK:CB	2.10	0.82
1:L4:321:UNK:O	1:L4:325:UNK:N	2.12	0.82
3:i4:22:UNK:O	3:i4:25:UNK:N	2.13	0.82
3:i1:22:UNK:O	3:i1:25:UNK:N	2.13	0.82
8:n3:10:UNK:O	8:n3:13:UNK:N	2.12	0.82
8:n5:10:UNK:O	8:n5:13:UNK:N	2.12	0.82
2:M5:210:UNK:HA	2:M5:268:UNK:CB	2.10	0.82
1:L6:321:UNK:O	1:L6:325:UNK:N	2.12	0.82
2:M6:210:UNK:HA	2:M6:268:UNK:CB	2.10	0.82
2:M1:281:UNK:O	2:M1:285:UNK:N	2.12	0.82
1:L1:321:UNK:O	1:L1:325:UNK:N	2.12	0.82
1:L2:435:UNK:CB	14:BB:1644:UNK:HA	2.09	0.82
2:M5:281:UNK:O	2:M5:285:UNK:N	2.12	0.82
7:U6:22:UNK:HA	14:BF:1635:UNK:CB	2.10	0.82
1:L1:435:UNK:CB	14:BA:1644:UNK:HA	2.09	0.82
1:L2:321:UNK:O	1:L2:325:UNK:N	2.12	0.82
1:L6:435:UNK:CB	14:BF:1644:UNK:HA	2.10	0.82
2:M3:281:UNK:O	2:M3:285:UNK:N	2.12	0.81
2:M4:210:UNK:HA	2:M4:268:UNK:CB	2.09	0.81
2:M1:210:UNK:HA	2:M1:268:UNK:CB	2.10	0.81
1:L2:77:UNK:HA	1:L2:78:UNK:CB	2.10	0.81
2:M2:210:UNK:HA	2:M2:268:UNK:CB	2.10	0.81
1:L5:321:UNK:O	1:L5:325:UNK:N	2.12	0.81
1:L5:435:UNK:CB	14:BE:1644:UNK:HA	2.09	0.81
1:L6:77:UNK:HA	1:L6:78:UNK:CB	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U5:22:UNK:HA	14:BE:1635:UNK:CB	2.10	0.81
8:n1:10:UNK:O	8:n1:13:UNK:N	2.12	0.81
2:M6:118:UNK:O	2:M6:122:UNK:N	2.14	0.81
2:M2:281:UNK:O	2:M2:285:UNK:N	2.12	0.81
3:i3:22:UNK:O	3:i3:25:UNK:N	2.13	0.81
1:L4:435:UNK:CB	14:BD:1644:UNK:HA	2.09	0.81
7:U4:22:UNK:HA	14:BD:1635:UNK:CB	2.10	0.81
5:s1:26:UNK:O	5:s1:27:UNK:C	2.28	0.81
14:BA:1609:UNK:CB	14:BA:1642:UNK:CA	2.59	0.81
1:L3:435:UNK:CB	14:BC:1644:UNK:HA	2.09	0.81
2:M3:118:UNK:O	2:M3:122:UNK:N	2.13	0.81
7:U3:22:UNK:HA	14:BC:1635:UNK:CB	2.10	0.81
8:n4:10:UNK:O	8:n4:13:UNK:N	2.12	0.81
7:U2:22:UNK:HA	14:BB:1635:UNK:CB	2.10	0.81
2:M4:118:UNK:O	2:M4:122:UNK:N	2.14	0.81
2:M4:281:UNK:O	2:M4:285:UNK:N	2.13	0.81
14:BE:1609:UNK:CB	14:BE:1642:UNK:CA	2.59	0.81
14:BB:1609:UNK:CB	14:BB:1642:UNK:CA	2.59	0.80
2:M5:118:UNK:O	2:M5:122:UNK:N	2.14	0.80
3:i5:22:UNK:O	3:i5:25:UNK:N	2.13	0.80
2:M1:118:UNK:O	2:M1:122:UNK:N	2.13	0.80
1:L2:321:UNK:O	1:L2:324:UNK:CA	2.30	0.80
1:L6:321:UNK:O	1:L6:324:UNK:CA	2.30	0.80
5:s6:26:UNK:O	5:s6:27:UNK:C	2.28	0.80
2:M2:118:UNK:O	2:M2:122:UNK:N	2.14	0.80
5:s2:26:UNK:O	5:s2:27:UNK:C	2.28	0.80
14:BF:1609:UNK:CB	14:BF:1642:UNK:CA	2.59	0.80
2:M1:108:UNK:HA	2:M1:111:UNK:CB	2.12	0.80
7:U3:35:UNK:CB	7:U3:38:UNK:CB	2.60	0.80
14:BD:1609:UNK:CB	14:BD:1642:UNK:CA	2.59	0.80
1:L5:77:UNK:HA	1:L5:78:UNK:CB	2.10	0.80
14:BC:1609:UNK:CB	14:BC:1642:UNK:CA	2.59	0.80
2:M4:108:UNK:HA	2:M4:111:UNK:CB	2.12	0.80
2:M6:241:UNK:O	2:M6:244:UNK:N	2.15	0.80
7:U1:22:UNK:HA	14:BA:1635:UNK:CB	2.10	0.79
2:M5:241:UNK:O	2:M5:244:UNK:N	2.15	0.79
2:M1:207:UNK:O	2:M1:208:UNK:CB	2.30	0.79
2:M1:241:UNK:O	2:M1:244:UNK:N	2.15	0.79
7:U2:35:UNK:CB	7:U2:38:UNK:CB	2.60	0.79
1:L3:225:UNK:CA	1:L3:229:UNK:CB	2.58	0.79
1:L3:321:UNK:O	1:L3:324:UNK:CA	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M6:207:UNK:O	2:M6:208:UNK:CB	2.30	0.79
1:L1:321:UNK:O	1:L1:324:UNK:CA	2.30	0.79
7:U1:35:UNK:CB	7:U1:38:UNK:CB	2.60	0.79
2:M5:108:UNK:HA	2:M5:111:UNK:CB	2.12	0.79
2:M2:108:UNK:HA	2:M2:111:UNK:CB	2.12	0.79
2:M4:241:UNK:O	2:M4:244:UNK:N	2.15	0.79
7:U5:21:UNK:C	14:BE:1635:UNK:CB	2.60	0.79
1:L1:225:UNK:CA	1:L1:229:UNK:CB	2.58	0.79
2:M3:108:UNK:HA	2:M3:111:UNK:CB	2.12	0.79
7:U5:35:UNK:CB	7:U5:38:UNK:CB	2.60	0.79
7:U3:21:UNK:C	14:BC:1635:UNK:CB	2.60	0.79
1:L5:321:UNK:O	1:L5:324:UNK:CA	2.29	0.79
2:M2:207:UNK:O	2:M2:208:UNK:CB	2.30	0.79
1:L4:321:UNK:O	1:L4:324:UNK:CA	2.29	0.79
2:M4:207:UNK:O	2:M4:208:UNK:CB	2.30	0.79
14:BD:1602:UNK:C	14:BD:1606:UNK:N	2.30	0.79
2:M6:108:UNK:HA	2:M6:111:UNK:CB	2.12	0.79
7:U2:21:UNK:C	14:BB:1635:UNK:CB	2.60	0.79
4:g4:16:UNK:O	4:g4:19:UNK:N	2.16	0.79
7:U1:21:UNK:C	14:BA:1635:UNK:CB	2.60	0.79
14:BD:547:UNK:CA	14:BE:1590:UNK:N	2.34	0.79
2:M5:207:UNK:O	2:M5:208:UNK:CB	2.30	0.79
7:U6:21:UNK:C	14:BF:1635:UNK:CB	2.60	0.79
4:g2:16:UNK:O	4:g2:19:UNK:N	2.16	0.78
7:U6:35:UNK:CB	7:U6:38:UNK:CB	2.60	0.78
2:M2:241:UNK:O	2:M2:244:UNK:N	2.15	0.78
5:j4:13:UNK:O	5:j4:16:UNK:N	2.17	0.78
4:g5:16:UNK:O	4:g5:19:UNK:N	2.16	0.78
2:M3:241:UNK:O	2:M3:244:UNK:N	2.15	0.78
7:U4:21:UNK:C	14:BD:1635:UNK:CB	2.60	0.78
7:U4:35:UNK:CB	7:U4:38:UNK:CB	2.60	0.78
1:L5:181:UNK:O	1:L5:182:UNK:C	2.32	0.78
1:L6:225:UNK:CA	1:L6:229:UNK:CB	2.58	0.78
5:j2:13:UNK:O	5:j2:16:UNK:N	2.17	0.78
1:L4:181:UNK:O	1:L4:182:UNK:C	2.32	0.78
4:g3:16:UNK:O	4:g3:19:UNK:N	2.16	0.78
2:M6:258:UNK:O	2:M6:262:UNK:N	2.17	0.78
6:l1:14:UNK:O	6:l1:17:UNK:CB	2.32	0.78
5:j3:13:UNK:O	5:j3:16:UNK:N	2.17	0.78
4:g6:16:UNK:O	4:g6:19:UNK:N	2.16	0.78
4:g1:16:UNK:O	4:g1:19:UNK:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:223:UNK:CB	1:L2:256:UNK:CB	2.62	0.78
2:M2:258:UNK:O	2:M2:262:UNK:N	2.17	0.78
6:l2:14:UNK:O	6:l2:17:UNK:CB	2.32	0.78
1:L3:142:UNK:HA	2:M3:370:UNK:CB	2.14	0.78
5:j1:13:UNK:O	5:j1:16:UNK:N	2.17	0.78
1:L3:181:UNK:O	1:L3:182:UNK:C	2.32	0.78
6:l4:14:UNK:O	6:l4:17:UNK:CB	2.32	0.78
1:L5:67:UNK:CB	1:L5:76:UNK:CB	2.62	0.78
1:L2:161:UNK:CA	1:L2:163:UNK:N	2.46	0.77
6:l3:14:UNK:O	6:l3:17:UNK:CB	2.32	0.77
1:L5:142:UNK:HA	2:M5:370:UNK:CB	2.14	0.77
2:M5:191:UNK:CB	2:M5:192:UNK:HA	2.14	0.77
5:s5:26:UNK:O	5:s5:27:UNK:C	2.28	0.77
2:M3:258:UNK:O	2:M3:262:UNK:N	2.17	0.77
2:M4:258:UNK:O	2:M4:262:UNK:N	2.17	0.77
6:l5:14:UNK:O	6:l5:17:UNK:CB	2.32	0.77
1:L1:223:UNK:CB	1:L1:256:UNK:CB	2.62	0.77
2:M1:258:UNK:O	2:M1:262:UNK:N	2.17	0.77
1:L2:181:UNK:O	1:L2:182:UNK:C	2.32	0.77
1:L6:142:UNK:HA	2:M6:370:UNK:CB	2.14	0.77
6:l6:14:UNK:O	6:l6:17:UNK:CB	2.32	0.77
2:M2:191:UNK:CB	2:M2:192:UNK:HA	2.14	0.77
14:BB:1602:UNK:C	14:BB:1606:UNK:N	2.30	0.77
1:L4:225:UNK:CA	1:L4:229:UNK:CB	2.58	0.77
2:M6:113:UNK:HA	2:M6:114:UNK:CB	2.13	0.77
1:L2:142:UNK:HA	2:M2:370:UNK:CB	2.14	0.77
1:L3:67:UNK:CB	1:L3:76:UNK:CB	2.62	0.77
1:L4:142:UNK:HA	2:M4:370:UNK:CB	2.14	0.77
1:L1:142:UNK:HA	2:M1:370:UNK:CB	2.14	0.77
1:L2:67:UNK:CB	1:L2:76:UNK:CB	2.62	0.77
1:L4:223:UNK:CB	1:L4:256:UNK:CB	2.62	0.77
5:s4:26:UNK:O	5:s4:27:UNK:C	2.29	0.77
1:L6:181:UNK:O	1:L6:182:UNK:C	2.32	0.77
1:L6:223:UNK:CB	1:L6:256:UNK:CB	2.62	0.77
1:L3:223:UNK:CB	1:L3:256:UNK:CB	2.62	0.77
2:M3:25:UNK:O	2:M3:28:UNK:N	2.18	0.77
1:L5:225:UNK:CA	1:L5:229:UNK:CB	2.58	0.77
2:M5:25:UNK:O	2:M5:28:UNK:N	2.18	0.77
2:M3:113:UNK:HA	2:M3:114:UNK:CB	2.13	0.76
2:M2:113:UNK:HA	2:M2:114:UNK:CB	2.13	0.76
2:M3:207:UNK:O	2:M3:208:UNK:CB	2.30	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M4:25:UNK:O	2:M4:28:UNK:N	2.18	0.76
1:L5:223:UNK:CB	1:L5:256:UNK:CB	2.62	0.76
2:M5:258:UNK:O	2:M5:262:UNK:N	2.17	0.76
1:L1:181:UNK:O	1:L1:182:UNK:C	2.32	0.76
2:M3:191:UNK:CB	2:M3:192:UNK:HA	2.14	0.76
1:L4:67:UNK:CB	1:L4:76:UNK:CB	2.62	0.76
2:M4:62:UNK:N	2:M4:63:UNK:HA	2.00	0.76
1:L6:67:UNK:CB	1:L6:76:UNK:CB	2.62	0.76
2:M6:25:UNK:O	2:M6:28:UNK:N	2.18	0.76
2:M2:62:UNK:N	2:M2:63:UNK:HA	2.00	0.76
2:M3:347:UNK:O	2:M3:351:UNK:CA	2.34	0.76
2:M4:447:UNK:O	2:M4:450:UNK:O	2.04	0.76
2:M1:113:UNK:HA	2:M1:114:UNK:CB	2.13	0.76
2:M1:347:UNK:O	2:M1:351:UNK:CA	2.34	0.76
1:L2:225:UNK:CA	1:L2:229:UNK:CB	2.59	0.76
2:M2:447:UNK:O	2:M2:450:UNK:O	2.04	0.76
5:j5:13:UNK:O	5:j5:16:UNK:N	2.17	0.76
14:BE:1602:UNK:C	14:BE:1606:UNK:N	2.30	0.76
2:M6:191:UNK:CB	2:M6:192:UNK:HA	2.14	0.76
1:L1:67:UNK:CB	1:L1:76:UNK:CB	2.62	0.76
2:M1:25:UNK:O	2:M1:28:UNK:N	2.18	0.76
2:M5:347:UNK:O	2:M5:351:UNK:CA	2.34	0.76
5:j6:13:UNK:O	5:j6:16:UNK:N	2.17	0.76
2:M1:62:UNK:N	2:M1:63:UNK:HA	2.00	0.76
14:BA:1602:UNK:C	14:BA:1606:UNK:N	2.30	0.76
2:M2:347:UNK:O	2:M2:351:UNK:CA	2.34	0.76
2:M4:191:UNK:CB	2:M4:192:UNK:HA	2.14	0.76
2:M4:347:UNK:O	2:M4:351:UNK:CA	2.34	0.76
1:L6:503:UNK:O	1:L6:507:UNK:N	2.19	0.76
1:L1:503:UNK:O	1:L1:507:UNK:N	2.19	0.76
2:M1:191:UNK:CB	2:M1:192:UNK:HA	2.14	0.76
1:L3:503:UNK:O	1:L3:507:UNK:N	2.19	0.76
2:M5:113:UNK:HA	2:M5:114:UNK:CB	2.13	0.76
1:L4:190:UNK:HA	1:L4:194:UNK:HA	1.68	0.76
1:L5:190:UNK:HA	1:L5:194:UNK:HA	1.68	0.76
2:M6:62:UNK:N	2:M6:63:UNK:HA	2.00	0.76
2:M1:447:UNK:O	2:M1:450:UNK:O	2.04	0.75
2:M4:113:UNK:HA	2:M4:114:UNK:CB	2.13	0.75
2:M3:447:UNK:O	2:M3:450:UNK:O	2.04	0.75
2:M4:372:UNK:O	2:M4:376:UNK:N	2.20	0.75
2:M5:372:UNK:O	2:M5:376:UNK:N	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M1:372:UNK:O	2:M1:376:UNK:N	2.20	0.75
2:M2:25:UNK:O	2:M2:28:UNK:N	2.18	0.75
2:M5:62:UNK:N	2:M5:63:UNK:HA	2.00	0.75
2:M6:347:UNK:O	2:M6:351:UNK:CA	2.34	0.75
1:L4:161:UNK:CA	1:L4:163:UNK:N	2.46	0.75
2:M6:447:UNK:O	2:M6:450:UNK:O	2.04	0.75
2:M5:447:UNK:O	2:M5:450:UNK:O	2.04	0.75
1:L4:503:UNK:O	1:L4:507:UNK:N	2.19	0.75
2:M3:62:UNK:N	2:M3:63:UNK:HA	2.00	0.75
1:L5:503:UNK:O	1:L5:507:UNK:N	2.19	0.75
2:M6:372:UNK:O	2:M6:376:UNK:N	2.20	0.75
5:j6:13:UNK:O	5:j6:14:UNK:C	2.34	0.75
2:M1:241:UNK:O	2:M1:242:UNK:C	2.35	0.75
1:L3:190:UNK:HA	1:L3:194:UNK:HA	1.68	0.75
2:M1:275:UNK:O	2:M1:278:UNK:CB	2.35	0.74
1:L2:190:UNK:HA	1:L2:194:UNK:HA	1.68	0.74
2:M2:87:UNK:CB	2:M2:88:UNK:HA	2.17	0.74
2:M2:275:UNK:O	2:M2:278:UNK:CB	2.35	0.74
5:j4:13:UNK:O	5:j4:14:UNK:C	2.34	0.74
2:M5:275:UNK:O	2:M5:278:UNK:CB	2.35	0.74
1:L1:190:UNK:HA	1:L1:194:UNK:HA	1.68	0.74
2:M2:372:UNK:O	2:M2:376:UNK:N	2.20	0.74
2:M3:275:UNK:O	2:M3:278:UNK:CB	2.35	0.74
2:M2:23:UNK:O	2:M2:25:UNK:N	2.21	0.74
5:s3:26:UNK:O	5:s3:27:UNK:C	2.28	0.74
1:L4:165:UNK:O	1:L4:169:UNK:N	2.20	0.74
2:M6:87:UNK:CB	2:M6:88:UNK:HA	2.17	0.74
2:M3:372:UNK:O	2:M3:376:UNK:N	2.20	0.74
1:L6:190:UNK:HA	1:L6:194:UNK:HA	1.68	0.74
1:L2:503:UNK:O	1:L2:507:UNK:N	2.19	0.74
1:L3:165:UNK:O	1:L3:169:UNK:N	2.21	0.74
2:M4:275:UNK:O	2:M4:278:UNK:CB	2.35	0.74
1:L5:165:UNK:O	1:L5:169:UNK:N	2.21	0.74
5:j1:13:UNK:O	5:j1:14:UNK:C	2.34	0.74
1:L3:207:UNK:HA	1:L3:208:UNK:CB	2.18	0.74
5:j5:13:UNK:O	5:j5:14:UNK:C	2.34	0.74
2:M6:241:UNK:O	2:M6:242:UNK:C	2.35	0.74
1:L1:165:UNK:O	1:L1:169:UNK:N	2.21	0.74
2:M1:87:UNK:CB	2:M1:88:UNK:HA	2.17	0.74
1:L2:71:UNK:O	1:L2:72:UNK:CB	2.36	0.74
1:L2:224:UNK:N	1:L2:256:UNK:CB	2.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M3:241:UNK:O	2:M3:242:UNK:C	2.35	0.74
5:j3:13:UNK:O	5:j3:14:UNK:C	2.34	0.74
1:L4:71:UNK:O	1:L4:72:UNK:CB	2.36	0.74
1:L4:224:UNK:N	1:L4:256:UNK:CB	2.51	0.74
1:L1:71:UNK:O	1:L1:72:UNK:CB	2.36	0.74
1:L1:161:UNK:CA	1:L1:163:UNK:N	2.46	0.74
2:M5:23:UNK:O	2:M5:25:UNK:N	2.21	0.74
2:M5:87:UNK:CB	2:M5:88:UNK:HA	2.17	0.74
2:M5:241:UNK:O	2:M5:242:UNK:C	2.35	0.74
2:M3:87:UNK:CB	2:M3:88:UNK:HA	2.17	0.73
1:L6:165:UNK:O	1:L6:169:UNK:N	2.20	0.73
1:L6:224:UNK:N	1:L6:256:UNK:CB	2.51	0.73
1:L2:207:UNK:HA	1:L2:208:UNK:CB	2.18	0.73
1:L2:239:UNK:O	1:L2:240:UNK:O	2.06	0.73
2:M3:23:UNK:O	2:M3:25:UNK:N	2.21	0.73
2:M3:27:UNK:O	2:M3:30:UNK:N	2.21	0.73
2:M6:23:UNK:O	2:M6:25:UNK:N	2.21	0.73
1:L1:207:UNK:HA	1:L1:208:UNK:CB	2.18	0.73
2:M4:87:UNK:CB	2:M4:88:UNK:HA	2.17	0.73
1:L5:207:UNK:HA	1:L5:208:UNK:CB	2.18	0.73
1:L1:223:UNK:C	1:L1:256:UNK:CB	2.67	0.73
1:L1:224:UNK:N	1:L1:256:UNK:CB	2.51	0.73
1:L1:239:UNK:O	1:L1:240:UNK:O	2.06	0.73
2:M1:23:UNK:O	2:M1:25:UNK:N	2.21	0.73
1:L2:223:UNK:C	1:L2:256:UNK:CB	2.66	0.73
2:M6:275:UNK:O	2:M6:278:UNK:CB	2.35	0.73
2:M1:27:UNK:O	2:M1:30:UNK:N	2.22	0.73
1:L5:476:UNK:C	1:L5:480:UNK:CB	2.63	0.73
10:t5:53:UNK:O	10:t5:56:UNK:O	2.07	0.73
1:L2:209:UNK:O	1:L2:212:UNK:CB	2.37	0.73
1:L3:209:UNK:O	1:L3:212:UNK:CB	2.37	0.73
1:L3:239:UNK:O	1:L3:240:UNK:O	2.06	0.73
2:M4:23:UNK:O	2:M4:25:UNK:N	2.21	0.73
1:L5:71:UNK:O	1:L5:72:UNK:CB	2.36	0.73
1:L6:209:UNK:O	1:L6:212:UNK:CB	2.37	0.73
1:L5:223:UNK:C	1:L5:256:UNK:CB	2.67	0.73
1:L5:209:UNK:O	1:L5:212:UNK:CB	2.37	0.73
3:f5:29:UNK:O	3:f5:30:UNK:CB	2.36	0.73
2:M2:27:UNK:O	2:M2:30:UNK:N	2.21	0.73
1:L4:223:UNK:C	1:L4:256:UNK:CB	2.67	0.73
1:L5:224:UNK:N	1:L5:256:UNK:CB	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:165:UNK:O	1:L2:169:UNK:N	2.21	0.73
2:M2:241:UNK:O	2:M2:242:UNK:C	2.35	0.73
1:L3:224:UNK:N	1:L3:256:UNK:CB	2.51	0.73
14:BD:1613:UNK:O	14:BD:1617:UNK:CB	2.37	0.73
1:L6:71:UNK:O	1:L6:72:UNK:CB	2.36	0.73
1:L6:223:UNK:C	1:L6:256:UNK:CB	2.67	0.73
3:f6:29:UNK:O	3:f6:30:UNK:CB	2.36	0.73
10:t6:53:UNK:O	10:t6:56:UNK:O	2.07	0.73
14:BF:1613:UNK:O	14:BF:1617:UNK:CB	2.37	0.73
10:t2:53:UNK:O	10:t2:56:UNK:O	2.07	0.72
1:L4:209:UNK:O	1:L4:212:UNK:CB	2.37	0.72
5:j1:21:UNK:O	5:j1:22:UNK:C	2.38	0.72
14:BA:1613:UNK:O	14:BA:1617:UNK:CB	2.37	0.72
1:L3:223:UNK:C	1:L3:256:UNK:CB	2.67	0.72
10:t3:53:UNK:O	10:t3:56:UNK:O	2.07	0.72
1:L1:209:UNK:O	1:L1:212:UNK:CB	2.37	0.72
1:L5:239:UNK:O	1:L5:240:UNK:O	2.06	0.72
2:M6:27:UNK:O	2:M6:30:UNK:N	2.21	0.72
10:t1:53:UNK:O	10:t1:56:UNK:O	2.07	0.72
1:L4:476:UNK:C	1:L4:480:UNK:CB	2.63	0.72
1:L2:67:UNK:CB	1:L2:76:UNK:CA	2.68	0.72
14:BB:1613:UNK:O	14:BB:1617:UNK:CB	2.37	0.72
2:M4:241:UNK:O	2:M4:242:UNK:C	2.35	0.72
2:M5:27:UNK:O	2:M5:30:UNK:N	2.21	0.72
2:M1:31:UNK:O	2:M1:32:UNK:C	2.37	0.72
1:L6:161:UNK:CA	1:L6:163:UNK:N	2.46	0.72
3:f3:29:UNK:O	3:f3:30:UNK:CB	2.36	0.72
5:j3:21:UNK:O	5:j3:22:UNK:C	2.38	0.72
2:M4:27:UNK:O	2:M4:30:UNK:N	2.21	0.72
1:L6:207:UNK:HA	1:L6:208:UNK:CB	2.18	0.72
2:M1:32:UNK:O	2:M1:35:UNK:N	2.23	0.72
1:L4:239:UNK:O	1:L4:240:UNK:O	2.06	0.72
3:f4:29:UNK:O	3:f4:30:UNK:CB	2.36	0.72
1:L3:67:UNK:CB	1:L3:76:UNK:CA	2.68	0.72
1:L3:71:UNK:O	1:L3:72:UNK:CB	2.36	0.72
2:M3:32:UNK:O	2:M3:35:UNK:N	2.23	0.72
14:BE:1613:UNK:O	14:BE:1617:UNK:CB	2.37	0.72
1:L6:239:UNK:O	1:L6:240:UNK:O	2.06	0.72
3:f2:29:UNK:O	3:f2:30:UNK:CB	2.36	0.72
10:t4:53:UNK:O	10:t4:56:UNK:O	2.07	0.72
1:L5:67:UNK:CB	1:L5:76:UNK:CA	2.68	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M6:32:UNK:O	2:M6:35:UNK:N	2.23	0.72
3:f1:29:UNK:O	3:f1:30:UNK:CB	2.36	0.71
14:BC:1613:UNK:O	14:BC:1617:UNK:CB	2.37	0.71
1:L4:67:UNK:CB	1:L4:76:UNK:CA	2.68	0.71
1:L4:182:UNK:O	1:L4:186:UNK:N	2.23	0.71
1:L4:207:UNK:HA	1:L4:208:UNK:CB	2.18	0.71
1:L5:182:UNK:O	1:L5:186:UNK:N	2.23	0.71
5:j4:21:UNK:O	5:j4:22:UNK:C	2.38	0.71
2:M3:279:UNK:CB	2:M3:280:UNK:HA	2.20	0.71
2:M4:279:UNK:CB	2:M4:280:UNK:HA	2.20	0.71
1:L3:476:UNK:C	1:L3:480:UNK:CB	2.63	0.71
4:g4:16:UNK:O	4:g4:17:UNK:C	2.38	0.71
1:L2:182:UNK:O	1:L2:186:UNK:N	2.23	0.71
5:j2:21:UNK:O	5:j2:22:UNK:C	2.38	0.71
5:j6:21:UNK:O	5:j6:22:UNK:C	2.38	0.71
4:g1:16:UNK:O	4:g1:17:UNK:C	2.38	0.71
5:j5:21:UNK:O	5:j5:22:UNK:C	2.38	0.71
2:M4:32:UNK:O	2:M4:35:UNK:N	2.23	0.71
1:L6:67:UNK:CB	1:L6:76:UNK:CA	2.68	0.71
1:L6:476:UNK:C	1:L6:480:UNK:CB	2.63	0.71
2:M6:279:UNK:CB	2:M6:280:UNK:HA	2.20	0.71
4:g6:16:UNK:O	4:g6:17:UNK:C	2.38	0.71
1:L1:67:UNK:CB	1:L1:76:UNK:CA	2.68	0.71
5:j2:13:UNK:O	5:j2:14:UNK:C	2.34	0.71
2:M2:32:UNK:O	2:M2:35:UNK:N	2.23	0.71
2:M2:279:UNK:CB	2:M2:280:UNK:HA	2.20	0.71
1:L6:182:UNK:O	1:L6:186:UNK:N	2.23	0.71
1:L1:476:UNK:C	1:L1:480:UNK:CB	2.63	0.70
1:L3:182:UNK:O	1:L3:186:UNK:N	2.23	0.70
1:L5:180:UNK:O	1:L5:181:UNK:C	2.37	0.70
2:M5:32:UNK:O	2:M5:35:UNK:N	2.23	0.70
1:L1:182:UNK:O	1:L1:186:UNK:N	2.23	0.70
1:L4:180:UNK:O	1:L4:181:UNK:C	2.37	0.70
1:L4:34:UNK:HA	1:L4:37:UNK:CB	2.22	0.70
1:L1:35:UNK:O	1:L1:39:UNK:N	2.25	0.70
1:L3:161:UNK:CA	1:L3:163:UNK:N	2.46	0.70
2:M5:31:UNK:O	2:M5:32:UNK:C	2.37	0.70
1:L5:35:UNK:O	1:L5:39:UNK:N	2.25	0.70
1:L5:161:UNK:CA	1:L5:163:UNK:N	2.46	0.70
5:p5:11:UNK:O	5:p5:14:UNK:N	2.25	0.70
1:L2:35:UNK:O	1:L2:39:UNK:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:p2:11:UNK:O	5:p2:14:UNK:N	2.25	0.70
2:M1:279:UNK:CB	2:M1:280:UNK:HA	2.20	0.70
4:g3:16:UNK:O	4:g3:17:UNK:C	2.38	0.70
1:L4:472:UNK:O	1:L4:475:UNK:N	2.25	0.70
2:M5:279:UNK:CB	2:M5:280:UNK:HA	2.20	0.70
1:L1:472:UNK:O	1:L1:475:UNK:N	2.25	0.70
1:L4:35:UNK:O	1:L4:39:UNK:N	2.25	0.70
5:p4:11:UNK:O	5:p4:14:UNK:N	2.25	0.70
2:M2:31:UNK:O	2:M2:32:UNK:C	2.37	0.70
2:M6:274:UNK:O	2:M6:278:UNK:CB	2.40	0.70
1:L3:35:UNK:O	1:L3:39:UNK:N	2.25	0.69
2:M3:274:UNK:O	2:M3:278:UNK:CB	2.40	0.69
1:L5:34:UNK:HA	1:L5:37:UNK:CB	2.22	0.69
5:p6:11:UNK:O	5:p6:14:UNK:N	2.25	0.69
2:M2:274:UNK:O	2:M2:278:UNK:CB	2.40	0.69
1:L3:34:UNK:HA	1:L3:37:UNK:CB	2.22	0.69
1:L1:151:UNK:O	1:L1:155:UNK:N	2.26	0.69
1:L3:180:UNK:O	1:L3:181:UNK:C	2.37	0.69
1:L4:151:UNK:O	1:L4:155:UNK:N	2.26	0.69
1:L1:34:UNK:HA	1:L1:37:UNK:CB	2.22	0.69
2:M1:274:UNK:O	2:M1:278:UNK:CB	2.40	0.69
2:M4:274:UNK:O	2:M4:278:UNK:CB	2.40	0.69
2:M5:21:UNK:O	2:M5:22:UNK:C	2.41	0.69
4:g5:16:UNK:O	4:g5:17:UNK:C	2.38	0.69
1:L5:151:UNK:O	1:L5:155:UNK:N	2.26	0.69
2:M5:274:UNK:O	2:M5:278:UNK:CB	2.40	0.69
1:L6:314:UNK:O	1:L6:317:UNK:CB	2.41	0.69
2:M6:31:UNK:O	2:M6:32:UNK:C	2.37	0.69
1:L1:180:UNK:O	1:L1:181:UNK:C	2.37	0.69
2:M1:21:UNK:O	2:M1:22:UNK:C	2.41	0.69
1:L2:314:UNK:O	1:L2:317:UNK:CB	2.41	0.69
1:L2:472:UNK:O	1:L2:475:UNK:N	2.25	0.69
2:M2:167:UNK:O	2:M2:171:UNK:N	2.26	0.69
4:g2:16:UNK:O	4:g2:17:UNK:C	2.38	0.69
1:L3:314:UNK:O	1:L3:317:UNK:CB	2.41	0.69
1:L3:369:UNK:O	1:L3:373:UNK:N	2.26	0.69
1:L3:472:UNK:O	1:L3:475:UNK:N	2.25	0.69
2:M3:21:UNK:O	2:M3:22:UNK:C	2.41	0.69
1:L4:321:UNK:CA	1:L4:324:UNK:CB	2.70	0.69
2:M4:21:UNK:O	2:M4:22:UNK:C	2.41	0.69
1:L5:314:UNK:O	1:L5:317:UNK:CB	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:369:UNK:O	1:L5:373:UNK:N	2.26	0.69
1:L6:35:UNK:O	1:L6:39:UNK:N	2.25	0.69
1:L6:151:UNK:O	1:L6:155:UNK:N	2.26	0.69
2:M6:167:UNK:O	2:M6:171:UNK:N	2.26	0.69
2:M3:167:UNK:O	2:M3:171:UNK:N	2.26	0.69
2:M4:167:UNK:O	2:M4:171:UNK:N	2.26	0.69
2:M1:167:UNK:O	2:M1:171:UNK:N	2.26	0.69
5:p1:11:UNK:O	5:p1:14:UNK:N	2.25	0.69
1:L2:34:UNK:HA	1:L2:37:UNK:CB	2.22	0.69
1:L1:314:UNK:O	1:L1:317:UNK:CB	2.41	0.68
1:L3:151:UNK:O	1:L3:155:UNK:N	2.26	0.68
1:L5:321:UNK:CA	1:L5:324:UNK:CB	2.70	0.68
2:M5:167:UNK:O	2:M5:171:UNK:N	2.26	0.68
1:L6:34:UNK:HA	1:L6:37:UNK:CB	2.22	0.68
1:L1:369:UNK:O	1:L1:373:UNK:N	2.26	0.68
2:M1:60:UNK:C	2:M1:63:UNK:N	2.57	0.68
7:U2:43:UNK:O	7:U2:47:UNK:N	2.26	0.68
1:L4:419:UNK:O	1:L4:422:UNK:CB	2.42	0.68
7:U5:43:UNK:O	7:U5:47:UNK:N	2.26	0.68
1:L1:321:UNK:CA	1:L1:324:UNK:CB	2.70	0.68
2:M1:60:UNK:C	2:M1:62:UNK:C	2.72	0.68
7:U4:43:UNK:O	7:U4:47:UNK:N	2.26	0.68
2:M2:21:UNK:O	2:M2:22:UNK:C	2.41	0.68
2:M3:60:UNK:C	2:M3:62:UNK:C	2.72	0.68
7:U3:43:UNK:O	7:U3:47:UNK:N	2.26	0.68
1:L4:314:UNK:O	1:L4:317:UNK:CB	2.41	0.68
2:M6:60:UNK:C	2:M6:62:UNK:C	2.72	0.68
7:U6:43:UNK:O	7:U6:47:UNK:N	2.26	0.68
5:p3:11:UNK:O	5:p3:14:UNK:N	2.25	0.68
1:L4:369:UNK:O	1:L4:373:UNK:N	2.26	0.68
2:M5:24:UNK:O	2:M5:27:UNK:CB	2.42	0.68
14:BE:1600:UNK:O	14:BE:1604:UNK:N	2.27	0.68
1:L6:472:UNK:O	1:L6:475:UNK:N	2.25	0.68
1:L1:419:UNK:O	1:L1:422:UNK:CB	2.42	0.68
1:L3:419:UNK:O	1:L3:422:UNK:CB	2.42	0.68
2:M4:24:UNK:O	2:M4:27:UNK:CB	2.42	0.68
2:M5:60:UNK:C	2:M5:63:UNK:N	2.57	0.68
14:BA:1600:UNK:O	14:BA:1604:UNK:N	2.27	0.68
1:L2:419:UNK:O	1:L2:422:UNK:CB	2.42	0.68
2:M2:60:UNK:C	2:M2:62:UNK:C	2.72	0.68
1:L3:46:UNK:O	1:L3:49:UNK:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BD:1600:UNK:O	14:BD:1604:UNK:N	2.27	0.68
1:L5:472:UNK:O	1:L5:475:UNK:N	2.25	0.68
2:M6:21:UNK:O	2:M6:22:UNK:C	2.41	0.68
2:M2:24:UNK:O	2:M2:27:UNK:CB	2.42	0.68
1:L6:46:UNK:O	1:L6:49:UNK:N	2.27	0.68
1:L6:369:UNK:O	1:L6:373:UNK:N	2.26	0.68
10:t6:34:UNK:O	10:t6:35:UNK:C	2.41	0.68
2:M1:24:UNK:O	2:M1:27:UNK:CB	2.42	0.68
1:L2:369:UNK:O	1:L2:373:UNK:N	2.26	0.68
1:L4:46:UNK:O	1:L4:49:UNK:N	2.27	0.68
2:M3:60:UNK:C	2:M3:63:UNK:N	2.57	0.68
14:BC:1600:UNK:O	14:BC:1604:UNK:N	2.27	0.68
1:L5:46:UNK:O	1:L5:49:UNK:N	2.27	0.68
2:M2:60:UNK:C	2:M2:63:UNK:N	2.57	0.67
2:M3:31:UNK:O	2:M3:32:UNK:C	2.37	0.67
8:n3:43:UNK:O	8:n3:44:UNK:C	2.42	0.67
7:U1:43:UNK:O	7:U1:47:UNK:N	2.26	0.67
1:L2:226:UNK:HA	1:L2:284:UNK:CB	2.25	0.67
2:M3:24:UNK:O	2:M3:27:UNK:CB	2.42	0.67
3:i3:26:UNK:O	3:i3:28:UNK:O	2.12	0.67
1:L4:226:UNK:HA	1:L4:284:UNK:CB	2.25	0.67
2:M4:32:UNK:O	2:M4:33:UNK:C	2.42	0.67
2:M6:32:UNK:O	2:M6:33:UNK:C	2.42	0.67
1:L1:281:UNK:CB	1:L1:315:UNK:HA	2.25	0.67
10:t2:34:UNK:O	10:t2:35:UNK:C	2.41	0.67
1:L3:321:UNK:CA	1:L3:324:UNK:CB	2.70	0.67
2:M4:60:UNK:C	2:M4:63:UNK:N	2.57	0.67
2:M4:60:UNK:C	2:M4:62:UNK:C	2.72	0.67
2:M5:32:UNK:O	2:M5:33:UNK:C	2.42	0.67
1:L6:321:UNK:CA	1:L6:324:UNK:CB	2.70	0.67
1:L6:419:UNK:O	1:L6:422:UNK:CB	2.42	0.67
2:M6:60:UNK:C	2:M6:63:UNK:N	2.57	0.67
10:t1:34:UNK:O	10:t1:35:UNK:C	2.42	0.67
14:BB:1600:UNK:O	14:BB:1604:UNK:N	2.27	0.67
2:M3:102:UNK:O	2:M3:106:UNK:CB	2.43	0.67
2:M5:60:UNK:C	2:M5:62:UNK:C	2.72	0.67
1:L2:151:UNK:O	1:L2:155:UNK:N	2.26	0.67
1:L2:281:UNK:CB	1:L2:315:UNK:HA	2.25	0.67
1:L2:321:UNK:CA	1:L2:324:UNK:CB	2.70	0.67
4:g3:11:UNK:O	4:g3:12:UNK:C	2.43	0.67
2:M4:31:UNK:O	2:M4:32:UNK:C	2.37	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M6:102:UNK:O	2:M6:106:UNK:CB	2.43	0.67
14:BF:1600:UNK:O	14:BF:1604:UNK:N	2.27	0.67
1:L2:178:UNK:CB	1:L2:222:UNK:CB	2.73	0.67
1:L5:281:UNK:CB	1:L5:315:UNK:HA	2.25	0.67
1:L6:180:UNK:O	1:L6:181:UNK:C	2.37	0.67
1:L1:46:UNK:O	1:L1:49:UNK:N	2.27	0.67
1:L2:180:UNK:O	1:L2:181:UNK:C	2.37	0.67
4:g2:11:UNK:O	4:g2:12:UNK:C	2.43	0.67
1:L3:226:UNK:HA	1:L3:284:UNK:CB	2.25	0.67
2:M4:278:UNK:O	2:M4:279:UNK:CB	2.43	0.67
4:g4:11:UNK:O	4:g4:12:UNK:C	2.43	0.67
12:v5:3:UNK:O	12:v5:4:UNK:C	2.41	0.67
2:M6:24:UNK:O	2:M6:27:UNK:CB	2.42	0.67
3:i1:26:UNK:O	3:i1:28:UNK:O	2.12	0.67
1:L2:46:UNK:O	1:L2:49:UNK:N	2.27	0.67
2:M3:278:UNK:O	2:M3:279:UNK:CB	2.43	0.67
10:t3:34:UNK:O	10:t3:35:UNK:C	2.42	0.67
12:v3:3:UNK:C	12:v3:5:UNK:N	2.54	0.67
1:L6:178:UNK:CB	1:L6:222:UNK:CB	2.73	0.67
1:L6:226:UNK:HA	1:L6:284:UNK:CB	2.25	0.67
1:L1:226:UNK:HA	1:L1:284:UNK:CB	2.25	0.67
1:L4:281:UNK:CB	1:L4:315:UNK:HA	2.25	0.67
2:M4:102:UNK:O	2:M4:106:UNK:CB	2.43	0.67
1:L5:419:UNK:O	1:L5:422:UNK:CB	2.42	0.67
8:n5:43:UNK:O	8:n5:44:UNK:C	2.42	0.67
1:L6:281:UNK:CB	1:L6:315:UNK:HA	2.25	0.67
8:n1:43:UNK:O	8:n1:44:UNK:C	2.42	0.67
12:v1:3:UNK:O	12:v1:4:UNK:C	2.41	0.67
1:L2:476:UNK:C	1:L2:480:UNK:CB	2.63	0.67
1:L3:178:UNK:CB	1:L3:222:UNK:CB	2.73	0.67
1:L3:321:UNK:C	1:L3:324:UNK:CB	2.73	0.67
2:M3:32:UNK:O	2:M3:33:UNK:C	2.42	0.67
1:L1:178:UNK:CB	1:L1:222:UNK:CB	2.73	0.66
1:L1:297:UNK:HA	1:L1:355:UNK:HA	1.77	0.66
1:L1:321:UNK:C	1:L1:324:UNK:CB	2.73	0.66
1:L2:321:UNK:C	1:L2:324:UNK:CB	2.73	0.66
3:i2:26:UNK:O	3:i2:28:UNK:O	2.12	0.66
5:p2:11:UNK:O	5:p2:12:UNK:C	2.43	0.66
1:L3:281:UNK:CB	1:L3:315:UNK:HA	2.25	0.66
4:g5:11:UNK:O	4:g5:12:UNK:C	2.43	0.66
8:n6:43:UNK:O	8:n6:44:UNK:C	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:v6:3:UNK:C	12:v6:5:UNK:N	2.54	0.66
1:L2:207:UNK:CB	1:L2:209:UNK:HA	2.25	0.66
1:L2:326:UNK:O	1:L2:330:UNK:N	2.29	0.66
1:L3:207:UNK:CB	1:L3:209:UNK:HA	2.25	0.66
3:i4:26:UNK:O	3:i4:28:UNK:O	2.12	0.66
3:i6:26:UNK:O	3:i6:28:UNK:O	2.12	0.66
4:g1:11:UNK:O	4:g1:12:UNK:C	2.43	0.66
8:n1:44:UNK:O	8:n1:48:UNK:N	2.29	0.66
1:L3:375:UNK:O	1:L3:376:UNK:C	2.43	0.66
1:L4:178:UNK:CB	1:L4:222:UNK:CB	2.73	0.66
1:L1:207:UNK:CB	1:L1:209:UNK:HA	2.26	0.66
8:n4:44:UNK:O	8:n4:48:UNK:N	2.29	0.66
2:M5:278:UNK:O	2:M5:279:UNK:CB	2.43	0.66
3:i5:26:UNK:O	3:i5:28:UNK:O	2.12	0.66
1:L6:207:UNK:CB	1:L6:209:UNK:HA	2.25	0.66
2:M6:278:UNK:O	2:M6:279:UNK:CB	2.43	0.66
5:p6:11:UNK:O	5:p6:12:UNK:C	2.43	0.66
2:M2:102:UNK:O	2:M2:106:UNK:CB	2.43	0.66
1:L4:326:UNK:O	1:L4:330:UNK:N	2.29	0.66
8:n4:43:UNK:O	8:n4:44:UNK:C	2.42	0.66
1:L5:178:UNK:CB	1:L5:222:UNK:CB	2.73	0.66
1:L6:61:UNK:HA	1:L6:80:UNK:CB	2.26	0.66
1:L6:326:UNK:O	1:L6:330:UNK:N	2.29	0.66
1:L2:61:UNK:HA	1:L2:80:UNK:CB	2.26	0.66
2:M5:102:UNK:O	2:M5:106:UNK:CB	2.43	0.66
8:n5:44:UNK:O	8:n5:48:UNK:N	2.29	0.66
12:v2:3:UNK:C	12:v2:5:UNK:N	2.54	0.66
1:L5:226:UNK:HA	1:L5:284:UNK:CB	2.25	0.66
1:L5:297:UNK:HA	1:L5:355:UNK:HA	1.77	0.66
1:L6:375:UNK:O	1:L6:376:UNK:C	2.43	0.66
8:n2:44:UNK:O	8:n2:48:UNK:N	2.29	0.66
1:L4:321:UNK:C	1:L4:324:UNK:CB	2.73	0.66
12:v4:3:UNK:C	12:v4:5:UNK:N	2.54	0.66
1:L5:321:UNK:C	1:L5:324:UNK:CB	2.73	0.66
2:M3:281:UNK:O	2:M3:284:UNK:N	2.29	0.66
8:n3:44:UNK:O	8:n3:48:UNK:N	2.29	0.66
1:L4:297:UNK:HA	1:L4:355:UNK:HA	1.77	0.66
2:M5:281:UNK:O	2:M5:284:UNK:N	2.29	0.66
8:n6:44:UNK:O	8:n6:48:UNK:N	2.29	0.66
2:M1:102:UNK:O	2:M1:106:UNK:CB	2.43	0.66
2:M1:281:UNK:O	2:M1:284:UNK:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L3:297:UNK:HA	1:L3:355:UNK:HA	1.77	0.66
10:t1:6:UNK:O	10:t1:7:UNK:C	2.44	0.65
2:M2:32:UNK:O	2:M2:33:UNK:C	2.42	0.65
1:L3:326:UNK:O	1:L3:330:UNK:N	2.29	0.65
2:M3:271:UNK:O	2:M3:272:UNK:C	2.45	0.65
1:L5:61:UNK:HA	1:L5:80:UNK:CB	2.26	0.65
1:L5:375:UNK:O	1:L5:376:UNK:C	2.43	0.65
10:t6:6:UNK:O	10:t6:7:UNK:C	2.44	0.65
1:L1:61:UNK:HA	1:L1:80:UNK:CB	2.26	0.65
5:p4:11:UNK:O	5:p4:12:UNK:C	2.43	0.65
1:L1:375:UNK:O	1:L1:376:UNK:C	2.43	0.65
4:g1:11:UNK:O	4:g1:14:UNK:N	2.30	0.65
2:M2:60:UNK:O	2:M2:62:UNK:O	2.15	0.65
8:n2:43:UNK:O	8:n2:44:UNK:C	2.42	0.65
2:M3:60:UNK:O	2:M3:62:UNK:O	2.15	0.65
1:L5:207:UNK:CB	1:L5:209:UNK:HA	2.26	0.65
1:L5:326:UNK:O	1:L5:330:UNK:N	2.29	0.65
2:M1:32:UNK:O	2:M1:33:UNK:C	2.42	0.65
2:M1:375:UNK:O	2:M1:379:UNK:N	2.30	0.65
2:M4:271:UNK:O	2:M4:272:UNK:C	2.45	0.65
12:v4:3:UNK:O	12:v4:4:UNK:C	2.41	0.65
4:g5:11:UNK:O	4:g5:14:UNK:N	2.30	0.65
2:M6:375:UNK:O	2:M6:379:UNK:N	2.30	0.65
5:p3:11:UNK:O	5:p3:12:UNK:C	2.43	0.65
1:L6:297:UNK:HA	1:L6:355:UNK:HA	1.78	0.65
1:L2:297:UNK:HA	1:L2:355:UNK:HA	1.77	0.65
2:M2:375:UNK:O	2:M2:379:UNK:N	2.30	0.65
4:g2:11:UNK:O	4:g2:14:UNK:N	2.30	0.65
1:L4:61:UNK:HA	1:L4:80:UNK:CB	2.26	0.65
1:L4:207:UNK:CB	1:L4:209:UNK:HA	2.26	0.65
1:L6:321:UNK:C	1:L6:324:UNK:CB	2.73	0.65
2:M6:281:UNK:O	2:M6:284:UNK:N	2.29	0.65
10:t6:21:UNK:O	10:t6:23:UNK:N	2.30	0.65
1:L2:375:UNK:O	1:L2:376:UNK:C	2.43	0.65
2:M2:180:UNK:O	2:M2:181:UNK:C	2.44	0.65
2:M2:278:UNK:O	2:M2:279:UNK:CB	2.43	0.65
2:M2:281:UNK:O	2:M2:284:UNK:N	2.29	0.65
10:t2:6:UNK:O	10:t2:7:UNK:C	2.44	0.65
2:M3:271:UNK:O	2:M3:274:UNK:N	2.30	0.65
12:v3:3:UNK:O	12:v3:4:UNK:C	2.41	0.65
4:g4:11:UNK:O	4:g4:14:UNK:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M6:180:UNK:O	2:M6:181:UNK:C	2.44	0.65
4:g6:11:UNK:O	4:g6:12:UNK:C	2.43	0.65
2:M1:60:UNK:O	2:M1:62:UNK:O	2.15	0.65
2:M2:271:UNK:O	2:M2:274:UNK:N	2.30	0.65
1:L4:375:UNK:O	1:L4:376:UNK:C	2.43	0.65
2:M5:271:UNK:O	2:M5:274:UNK:N	2.30	0.65
2:M5:375:UNK:O	2:M5:379:UNK:N	2.30	0.65
2:M6:60:UNK:O	2:M6:62:UNK:O	2.15	0.65
10:t2:21:UNK:O	10:t2:23:UNK:N	2.30	0.65
2:M3:180:UNK:O	2:M3:181:UNK:C	2.44	0.65
4:g6:11:UNK:O	4:g6:14:UNK:N	2.30	0.65
4:g3:11:UNK:O	4:g3:14:UNK:N	2.30	0.65
2:M6:32:UNK:O	2:M6:34:UNK:N	2.30	0.65
2:M1:180:UNK:O	2:M1:181:UNK:C	2.44	0.64
2:M1:278:UNK:O	2:M1:279:UNK:CB	2.43	0.64
2:M2:32:UNK:O	2:M2:34:UNK:N	2.30	0.64
2:M4:32:UNK:O	2:M4:34:UNK:N	2.30	0.64
2:M6:271:UNK:O	2:M6:274:UNK:N	2.30	0.64
1:L1:210:UNK:O	1:L1:211:UNK:C	2.45	0.64
1:L1:326:UNK:O	1:L1:330:UNK:N	2.29	0.64
1:L3:420:UNK:O	1:L3:424:UNK:N	2.31	0.64
2:M3:32:UNK:O	2:M3:34:UNK:N	2.30	0.64
2:M3:432:UNK:O	2:M3:435:UNK:CB	2.45	0.64
14:BC:1590:UNK:CB	14:BF:547:UNK:CB	2.75	0.64
2:M4:60:UNK:O	2:M4:62:UNK:O	2.15	0.64
2:M4:382:UNK:O	2:M4:385:UNK:N	2.31	0.64
2:M5:32:UNK:O	2:M5:34:UNK:N	2.30	0.64
8:n5:25:UNK:O	8:n5:26:UNK:C	2.45	0.64
10:t5:6:UNK:O	10:t5:7:UNK:C	2.44	0.64
2:M1:271:UNK:O	2:M1:274:UNK:N	2.30	0.64
2:M1:342:UNK:O	2:M1:343:UNK:CB	2.45	0.64
2:M1:382:UNK:O	2:M1:385:UNK:N	2.31	0.64
1:L2:420:UNK:O	1:L2:424:UNK:N	2.31	0.64
1:L3:61:UNK:HA	1:L3:80:UNK:CB	2.26	0.64
2:M3:375:UNK:O	2:M3:379:UNK:N	2.30	0.64
10:t3:6:UNK:O	10:t3:7:UNK:C	2.44	0.64
2:M4:180:UNK:O	2:M4:181:UNK:C	2.44	0.64
2:M4:375:UNK:O	2:M4:379:UNK:N	2.30	0.64
10:t4:21:UNK:O	10:t4:23:UNK:N	2.30	0.64
10:t4:34:UNK:O	10:t4:35:UNK:C	2.41	0.64
1:L1:420:UNK:O	1:L1:424:UNK:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M3:281:UNK:O	2:M3:284:UNK:CA	2.46	0.64
10:t3:21:UNK:O	10:t3:23:UNK:N	2.30	0.64
2:M4:271:UNK:O	2:M4:274:UNK:N	2.30	0.64
1:L6:420:UNK:O	1:L6:424:UNK:N	2.31	0.64
2:M6:281:UNK:O	2:M6:284:UNK:CA	2.46	0.64
1:L1:209:UNK:O	1:L1:212:UNK:CA	2.46	0.64
1:L2:209:UNK:O	1:L2:212:UNK:CA	2.46	0.64
2:M6:432:UNK:O	2:M6:435:UNK:CB	2.45	0.64
2:M1:281:UNK:O	2:M1:284:UNK:CA	2.46	0.64
2:M2:382:UNK:O	2:M2:385:UNK:N	2.31	0.64
14:BC:1588:UNK:H	14:BF:547:UNK:CB	2.07	0.64
2:M4:281:UNK:O	2:M4:284:UNK:N	2.29	0.64
2:M5:180:UNK:O	2:M5:181:UNK:C	2.44	0.64
10:t5:21:UNK:O	10:t5:23:UNK:N	2.30	0.64
12:v5:3:UNK:C	12:v5:5:UNK:N	2.54	0.64
2:M6:271:UNK:O	2:M6:272:UNK:C	2.45	0.64
2:M6:342:UNK:O	2:M6:343:UNK:CB	2.45	0.64
2:M6:382:UNK:O	2:M6:385:UNK:N	2.31	0.64
12:v6:3:UNK:O	12:v6:4:UNK:C	2.41	0.64
2:M1:123:UNK:O	2:M1:126:UNK:N	2.31	0.64
2:M3:123:UNK:O	2:M3:126:UNK:N	2.31	0.64
2:M4:432:UNK:O	2:M4:435:UNK:CB	2.45	0.64
8:n4:25:UNK:O	8:n4:26:UNK:C	2.45	0.64
2:M5:123:UNK:O	2:M5:126:UNK:N	2.31	0.64
2:M5:281:UNK:O	2:M5:284:UNK:CA	2.46	0.64
2:M5:432:UNK:O	2:M5:435:UNK:CB	2.45	0.64
10:t1:21:UNK:O	10:t1:23:UNK:N	2.30	0.64
2:M2:432:UNK:O	2:M2:435:UNK:CB	2.46	0.64
1:L4:209:UNK:O	1:L4:212:UNK:CA	2.46	0.64
1:L5:420:UNK:O	1:L5:424:UNK:N	2.31	0.64
2:M5:382:UNK:O	2:M5:385:UNK:N	2.31	0.64
2:M1:271:UNK:O	2:M1:272:UNK:C	2.45	0.64
8:n2:25:UNK:O	8:n2:26:UNK:C	2.45	0.64
1:L3:209:UNK:O	1:L3:212:UNK:CA	2.46	0.64
2:M3:382:UNK:O	2:M3:385:UNK:N	2.31	0.64
1:L4:376:UNK:O	1:L4:377:UNK:C	2.46	0.64
2:M4:281:UNK:O	2:M4:284:UNK:CA	2.46	0.64
1:L6:209:UNK:O	1:L6:212:UNK:CA	2.46	0.64
2:M1:432:UNK:O	2:M1:435:UNK:CB	2.46	0.63
2:M4:123:UNK:O	2:M4:126:UNK:N	2.31	0.63
2:M5:271:UNK:O	2:M5:272:UNK:C	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n1:25:UNK:O	8:n1:26:UNK:C	2.45	0.63
1:L4:420:UNK:O	1:L4:424:UNK:N	2.31	0.63
1:L6:210:UNK:O	1:L6:211:UNK:C	2.45	0.63
1:L6:376:UNK:O	1:L6:377:UNK:C	2.46	0.63
2:M1:32:UNK:O	2:M1:34:UNK:N	2.30	0.63
10:t4:6:UNK:O	10:t4:7:UNK:C	2.44	0.63
2:M6:123:UNK:O	2:M6:126:UNK:N	2.31	0.63
1:L1:376:UNK:O	1:L1:377:UNK:C	2.46	0.63
2:M1:68:UNK:O	2:M1:70:UNK:N	2.32	0.63
2:M2:342:UNK:O	2:M2:343:UNK:CB	2.45	0.63
1:L4:210:UNK:O	1:L4:211:UNK:C	2.45	0.63
2:M4:68:UNK:O	2:M4:70:UNK:N	2.32	0.63
2:M5:60:UNK:O	2:M5:62:UNK:O	2.15	0.63
2:M6:441:UNK:O	2:M6:445:UNK:N	2.32	0.63
5:p1:11:UNK:O	5:p1:12:UNK:C	2.43	0.63
2:M2:68:UNK:O	2:M2:70:UNK:N	2.32	0.63
12:v2:3:UNK:O	12:v2:4:UNK:C	2.41	0.63
2:M3:342:UNK:O	2:M3:343:UNK:CB	2.45	0.63
7:U5:62:UNK:CB	7:U5:66:UNK:CB	2.77	0.63
10:t5:34:UNK:O	10:t5:35:UNK:C	2.42	0.63
2:M4:441:UNK:O	2:M4:445:UNK:N	2.32	0.63
2:M1:441:UNK:O	2:M1:445:UNK:N	2.32	0.63
2:M2:271:UNK:O	2:M2:272:UNK:C	2.45	0.63
7:U3:62:UNK:CB	7:U3:66:UNK:CB	2.77	0.63
8:n3:25:UNK:O	8:n3:26:UNK:C	2.45	0.63
2:M5:342:UNK:O	2:M5:343:UNK:CB	2.45	0.63
14:BA:1637:UNK:HA	14:BA:1639:UNK:N	2.14	0.62
2:M2:123:UNK:O	2:M2:126:UNK:N	2.31	0.62
2:M2:441:UNK:O	2:M2:445:UNK:N	2.32	0.62
14:BF:1637:UNK:HA	14:BF:1639:UNK:N	2.14	0.62
3:h1:9:UNK:O	3:h1:12:UNK:N	2.32	0.62
7:U1:62:UNK:CB	7:U1:66:UNK:CB	2.77	0.62
1:L2:116:UNK:O	1:L2:117:UNK:C	2.45	0.62
2:M2:281:UNK:O	2:M2:284:UNK:CA	2.46	0.62
7:U4:62:UNK:CB	7:U4:66:UNK:CB	2.77	0.62
14:BD:1637:UNK:HA	14:BD:1639:UNK:N	2.14	0.62
8:n5:43:UNK:C	8:n5:45:UNK:N	2.59	0.62
5:p5:11:UNK:O	5:p5:12:UNK:C	2.43	0.62
1:L2:376:UNK:O	1:L2:377:UNK:C	2.46	0.62
2:M5:441:UNK:O	2:M5:445:UNK:N	2.32	0.62
14:BB:1637:UNK:HA	14:BB:1639:UNK:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h4:9:UNK:O	3:h4:12:UNK:N	2.32	0.62
3:h2:9:UNK:O	3:h2:12:UNK:N	2.32	0.62
1:L5:209:UNK:O	1:L5:212:UNK:CA	2.46	0.62
8:n2:21:UNK:O	8:n2:22:UNK:CB	2.48	0.62
8:n6:25:UNK:O	8:n6:26:UNK:C	2.45	0.62
2:M3:441:UNK:O	2:M3:445:UNK:N	2.32	0.62
1:L5:116:UNK:O	1:L5:117:UNK:C	2.45	0.62
1:L5:210:UNK:O	1:L5:211:UNK:C	2.45	0.62
1:L5:383:UNK:O	1:L5:389:UNK:CB	2.48	0.62
3:h5:9:UNK:O	3:h5:12:UNK:N	2.32	0.62
7:U2:62:UNK:CB	7:U2:66:UNK:CB	2.77	0.62
1:L3:383:UNK:O	1:L3:389:UNK:CB	2.48	0.62
3:h3:9:UNK:O	3:h3:12:UNK:N	2.32	0.62
1:L5:376:UNK:O	1:L5:377:UNK:C	2.46	0.62
1:L1:376:UNK:O	1:L1:378:UNK:N	2.33	0.62
2:M1:26:UNK:O	2:M1:27:UNK:C	2.47	0.62
2:M4:342:UNK:O	2:M4:343:UNK:CB	2.45	0.62
1:L6:383:UNK:O	1:L6:389:UNK:CB	2.48	0.62
1:L3:376:UNK:O	1:L3:377:UNK:C	2.46	0.62
2:M3:68:UNK:O	2:M3:70:UNK:N	2.32	0.62
8:n3:21:UNK:O	8:n3:22:UNK:CB	2.48	0.62
1:L4:116:UNK:O	1:L4:117:UNK:C	2.45	0.62
14:BE:1637:UNK:HA	14:BE:1639:UNK:N	2.14	0.62
12:v1:3:UNK:C	12:v1:5:UNK:N	2.54	0.61
1:L3:116:UNK:O	1:L3:117:UNK:C	2.45	0.61
14:BE:1614:UNK:O	14:BE:1615:UNK:C	2.48	0.61
7:U6:62:UNK:CB	7:U6:66:UNK:CB	2.77	0.61
2:M1:168:UNK:CB	2:M1:174:UNK:HA	2.30	0.61
8:n4:21:UNK:O	8:n4:22:UNK:CB	2.48	0.61
2:M6:168:UNK:CB	2:M6:174:UNK:HA	2.30	0.61
1:L5:376:UNK:O	1:L5:378:UNK:N	2.33	0.61
1:L6:376:UNK:O	1:L6:378:UNK:N	2.33	0.61
3:h6:9:UNK:O	3:h6:12:UNK:N	2.32	0.61
1:L2:376:UNK:O	1:L2:378:UNK:N	2.33	0.61
1:L3:210:UNK:O	1:L3:211:UNK:C	2.45	0.61
1:L3:376:UNK:O	1:L3:378:UNK:N	2.33	0.61
8:n3:5:UNK:O	8:n3:6:UNK:C	2.48	0.61
1:L4:383:UNK:O	1:L4:389:UNK:CB	2.48	0.61
14:BD:1614:UNK:O	14:BD:1615:UNK:C	2.48	0.61
14:BA:1614:UNK:O	14:BA:1615:UNK:C	2.48	0.61
1:L2:210:UNK:O	1:L2:211:UNK:C	2.45	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M3:80:UNK:O	2:M3:81:UNK:C	2.49	0.61
13:w3:3:UNK:O	13:w3:6:UNK:N	2.33	0.61
1:L4:376:UNK:O	1:L4:378:UNK:N	2.33	0.61
1:L1:383:UNK:O	1:L1:389:UNK:CB	2.48	0.61
13:w1:3:UNK:O	13:w1:6:UNK:N	2.34	0.61
1:L2:383:UNK:O	1:L2:389:UNK:CB	2.48	0.61
8:n5:21:UNK:O	8:n5:22:UNK:CB	2.48	0.61
8:n6:43:UNK:C	8:n6:45:UNK:N	2.60	0.61
8:n1:21:UNK:O	8:n1:22:UNK:CB	2.48	0.61
8:n1:43:UNK:C	8:n1:45:UNK:N	2.60	0.61
13:w2:3:UNK:O	13:w2:6:UNK:N	2.33	0.61
2:M5:68:UNK:O	2:M5:70:UNK:N	2.32	0.61
8:n6:21:UNK:O	8:n6:22:UNK:CB	2.48	0.61
2:M2:168:UNK:CB	2:M2:174:UNK:HA	2.30	0.61
14:BB:1614:UNK:O	14:BB:1615:UNK:C	2.48	0.61
2:M3:168:UNK:CB	2:M3:174:UNK:HA	2.30	0.61
8:n3:43:UNK:C	8:n3:45:UNK:N	2.60	0.61
5:s3:23:UNK:O	5:s3:26:UNK:CB	2.49	0.61
2:M4:168:UNK:CB	2:M4:174:UNK:HA	2.30	0.61
13:w4:3:UNK:O	13:w4:6:UNK:N	2.33	0.61
5:s6:23:UNK:O	5:s6:26:UNK:CB	2.49	0.61
14:BC:1591:UNK:CB	14:BF:547:UNK:O	2.49	0.61
2:M6:68:UNK:O	2:M6:70:UNK:N	2.32	0.61
6:l1:19:UNK:O	6:l1:22:UNK:O	2.19	0.60
2:M3:26:UNK:O	2:M3:27:UNK:C	2.47	0.60
14:BC:1614:UNK:O	14:BC:1615:UNK:C	2.49	0.60
2:M5:68:UNK:O	2:M5:71:UNK:N	2.34	0.60
8:n3:9:UNK:O	8:n3:12:UNK:N	2.35	0.60
8:n4:52:UNK:O	8:n4:55:UNK:N	2.35	0.60
2:M5:80:UNK:O	2:M5:81:UNK:C	2.49	0.60
2:M5:113:UNK:HA	2:M5:114:UNK:C	2.31	0.60
2:M6:113:UNK:HA	2:M6:114:UNK:C	2.31	0.60
2:M2:137:UNK:O	2:M2:138:UNK:CB	2.50	0.60
5:s2:23:UNK:O	5:s2:26:UNK:CB	2.49	0.60
14:BC:1637:UNK:HA	14:BC:1639:UNK:N	2.14	0.60
6:l4:19:UNK:O	6:l4:22:UNK:O	2.20	0.60
8:n4:9:UNK:O	8:n4:12:UNK:N	2.35	0.60
1:L1:116:UNK:O	1:L1:117:UNK:C	2.45	0.60
1:L1:502:UNK:O	1:L1:506:UNK:N	2.35	0.60
2:M4:137:UNK:O	2:M4:138:UNK:CB	2.50	0.60
5:s4:23:UNK:O	5:s4:26:UNK:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M6:26:UNK:O	2:M6:27:UNK:C	2.47	0.60
8:n6:9:UNK:O	8:n6:12:UNK:N	2.35	0.60
5:s1:23:UNK:O	5:s1:26:UNK:CB	2.49	0.60
1:L2:502:UNK:O	1:L2:506:UNK:N	2.35	0.60
2:M2:26:UNK:O	2:M2:27:UNK:C	2.47	0.60
8:n2:43:UNK:C	8:n2:45:UNK:N	2.60	0.60
10:t2:20:UNK:O	10:t2:21:UNK:CB	2.50	0.60
2:M1:68:UNK:O	2:M1:71:UNK:N	2.34	0.60
8:n1:9:UNK:O	8:n1:12:UNK:N	2.35	0.60
8:n1:52:UNK:O	8:n1:55:UNK:N	2.35	0.60
2:M5:168:UNK:CB	2:M5:174:UNK:HA	2.30	0.60
5:s5:23:UNK:O	5:s5:26:UNK:CB	2.49	0.60
1:L6:502:UNK:O	1:L6:506:UNK:N	2.35	0.60
13:w6:3:UNK:O	13:w6:6:UNK:N	2.33	0.60
14:BC:1614:UNK:C	14:BC:1617:UNK:N	2.65	0.60
2:M4:113:UNK:HA	2:M4:114:UNK:C	2.31	0.60
1:L5:321:UNK:C	1:L5:324:UNK:N	2.65	0.60
2:M5:26:UNK:O	2:M5:27:UNK:C	2.47	0.60
3:i6:23:UNK:O	3:i6:26:UNK:CB	2.50	0.60
8:n6:52:UNK:O	8:n6:55:UNK:N	2.35	0.60
10:t6:20:UNK:O	10:t6:21:UNK:CB	2.50	0.60
14:BF:1614:UNK:C	14:BF:1617:UNK:N	2.65	0.60
2:M3:68:UNK:O	2:M3:71:UNK:N	2.34	0.60
1:L4:321:UNK:C	1:L4:324:UNK:N	2.64	0.60
6:l5:19:UNK:O	6:l5:22:UNK:O	2.20	0.60
10:t5:20:UNK:O	10:t5:21:UNK:CB	2.50	0.60
13:w5:3:UNK:O	13:w5:6:UNK:N	2.33	0.60
2:M6:137:UNK:O	2:M6:138:UNK:CB	2.50	0.60
8:n6:5:UNK:O	8:n6:6:UNK:C	2.48	0.60
2:M1:80:UNK:O	2:M1:81:UNK:C	2.49	0.60
1:L2:321:UNK:C	1:L2:324:UNK:N	2.64	0.60
2:M2:113:UNK:HA	2:M2:114:UNK:C	2.31	0.60
2:M2:324:UNK:O	2:M2:328:UNK:CB	2.50	0.60
8:n2:5:UNK:O	8:n2:6:UNK:C	2.48	0.60
8:n2:9:UNK:O	8:n2:12:UNK:N	2.35	0.60
14:BB:1614:UNK:C	14:BB:1617:UNK:N	2.65	0.60
1:L3:502:UNK:O	1:L3:506:UNK:N	2.35	0.60
2:M3:324:UNK:O	2:M3:328:UNK:CB	2.50	0.60
3:i4:23:UNK:O	3:i4:26:UNK:CB	2.50	0.60
12:v5:20:UNK:O	12:v5:24:UNK:N	2.35	0.60
1:L6:463:UNK:O	1:L6:467:UNK:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:321:UNK:C	1:L1:324:UNK:N	2.64	0.60
8:n1:5:UNK:O	8:n1:6:UNK:C	2.48	0.60
12:v1:20:UNK:O	12:v1:24:UNK:N	2.35	0.60
2:M2:356:UNK:O	2:M2:360:UNK:N	2.35	0.60
1:L3:463:UNK:O	1:L3:467:UNK:N	2.35	0.60
12:v3:20:UNK:O	12:v3:24:UNK:N	2.35	0.60
1:L5:502:UNK:O	1:L5:506:UNK:N	2.35	0.60
2:M5:137:UNK:O	2:M5:138:UNK:CB	2.50	0.60
2:M2:80:UNK:O	2:M2:81:UNK:C	2.49	0.59
2:M3:137:UNK:O	2:M3:138:UNK:CB	2.50	0.59
1:L5:463:UNK:O	1:L5:467:UNK:N	2.35	0.59
3:i5:23:UNK:O	3:i5:26:UNK:CB	2.50	0.59
8:n5:52:UNK:O	8:n5:55:UNK:N	2.35	0.59
2:M6:324:UNK:O	2:M6:328:UNK:CB	2.50	0.59
2:M6:356:UNK:O	2:M6:360:UNK:N	2.35	0.59
1:L1:475:UNK:O	1:L1:479:UNK:CB	2.51	0.59
2:M1:324:UNK:O	2:M1:328:UNK:CB	2.50	0.59
8:n2:52:UNK:O	8:n2:55:UNK:N	2.34	0.59
1:L3:128:UNK:O	1:L3:131:UNK:N	2.36	0.59
1:L3:321:UNK:C	1:L3:324:UNK:N	2.64	0.59
8:n3:52:UNK:O	8:n3:55:UNK:N	2.35	0.59
1:L4:463:UNK:O	1:L4:467:UNK:N	2.35	0.59
1:L5:475:UNK:O	1:L5:479:UNK:CB	2.51	0.59
1:L6:321:UNK:C	1:L6:324:UNK:N	2.64	0.59
2:M6:68:UNK:O	2:M6:71:UNK:N	2.34	0.59
2:M6:80:UNK:O	2:M6:81:UNK:C	2.49	0.59
2:M1:108:UNK:CA	2:M1:111:UNK:CB	2.80	0.59
1:L2:211:UNK:O	1:L2:214:UNK:CB	2.51	0.59
1:L2:316:UNK:O	1:L2:319:UNK:CB	2.51	0.59
1:L4:316:UNK:O	1:L4:319:UNK:CB	2.51	0.59
1:L4:502:UNK:O	1:L4:506:UNK:N	2.35	0.59
14:BF:1614:UNK:O	14:BF:1615:UNK:C	2.48	0.59
1:L1:128:UNK:O	1:L1:131:UNK:N	2.36	0.59
2:M1:356:UNK:O	2:M1:360:UNK:N	2.35	0.59
2:M2:68:UNK:O	2:M2:71:UNK:N	2.34	0.59
2:M2:108:UNK:CA	2:M2:111:UNK:CB	2.80	0.59
3:i2:23:UNK:O	3:i2:26:UNK:CB	2.50	0.59
5:j2:14:UNK:O	5:j2:17:UNK:CB	2.51	0.59
6:l2:19:UNK:O	6:l2:22:UNK:O	2.19	0.59
12:v2:20:UNK:O	12:v2:24:UNK:N	2.35	0.59
10:t3:20:UNK:O	10:t3:21:UNK:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M4:68:UNK:O	2:M4:71:UNK:N	2.34	0.59
2:M4:356:UNK:O	2:M4:360:UNK:N	2.35	0.59
5:k4:23:UNK:O	5:k4:26:UNK:CB	2.51	0.59
12:v4:20:UNK:O	12:v4:24:UNK:N	2.35	0.59
8:n5:9:UNK:O	8:n5:12:UNK:N	2.35	0.59
2:M1:113:UNK:HA	2:M1:114:UNK:C	2.31	0.59
2:M1:137:UNK:O	2:M1:138:UNK:CB	2.50	0.59
1:L2:463:UNK:O	1:L2:467:UNK:N	2.35	0.59
1:L3:211:UNK:O	1:L3:214:UNK:CB	2.51	0.59
2:M4:80:UNK:O	2:M4:81:UNK:C	2.49	0.59
2:M5:108:UNK:CA	2:M5:111:UNK:CB	2.81	0.59
5:k2:23:UNK:O	5:k2:26:UNK:CB	2.51	0.59
5:k3:23:UNK:O	5:k3:26:UNK:CB	2.51	0.59
6:l3:19:UNK:O	6:l3:22:UNK:O	2.19	0.59
1:L4:475:UNK:O	1:L4:479:UNK:CB	2.51	0.59
14:BD:547:UNK:O	14:BE:1588:UNK:C	2.50	0.59
10:t5:9:UNK:O	10:t5:12:UNK:N	2.36	0.59
14:BE:1614:UNK:C	14:BE:1617:UNK:N	2.65	0.59
1:L6:316:UNK:O	1:L6:319:UNK:CB	2.51	0.59
6:l6:19:UNK:O	6:l6:22:UNK:O	2.19	0.59
1:L1:463:UNK:O	1:L1:467:UNK:N	2.35	0.59
3:i1:23:UNK:O	3:i1:26:UNK:CB	2.50	0.59
2:M3:113:UNK:HA	2:M3:114:UNK:C	2.31	0.59
2:M4:108:UNK:CA	2:M4:111:UNK:CB	2.80	0.59
5:j4:14:UNK:O	5:j4:17:UNK:CB	2.51	0.59
8:n4:43:UNK:C	8:n4:45:UNK:N	2.60	0.59
5:j6:14:UNK:O	5:j6:17:UNK:CB	2.51	0.59
7:U6:9:UNK:O	7:U6:12:UNK:CB	2.51	0.59
5:j1:14:UNK:O	5:j1:17:UNK:CB	2.51	0.59
14:BA:1614:UNK:C	14:BA:1617:UNK:N	2.65	0.59
1:L3:316:UNK:O	1:L3:319:UNK:CB	2.51	0.59
2:M4:324:UNK:O	2:M4:328:UNK:CB	2.50	0.59
1:L5:211:UNK:O	1:L5:214:UNK:CB	2.51	0.59
2:M5:94:UNK:O	2:M5:95:UNK:C	2.48	0.59
2:M6:68:UNK:C	2:M6:70:UNK:N	2.66	0.59
10:t3:9:UNK:O	10:t3:12:UNK:N	2.36	0.59
12:v6:20:UNK:O	12:v6:24:UNK:N	2.35	0.59
1:L1:316:UNK:O	1:L1:319:UNK:CB	2.51	0.59
7:U1:9:UNK:O	7:U1:12:UNK:CB	2.51	0.59
7:U2:9:UNK:O	7:U2:12:UNK:CB	2.51	0.59
2:M3:42:UNK:O	2:M3:44:UNK:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i3:23:UNK:O	3:i3:26:UNK:CB	2.50	0.59
7:U4:9:UNK:O	7:U4:12:UNK:CB	2.51	0.59
5:j5:14:UNK:O	5:j5:17:UNK:CB	2.51	0.59
1:L6:128:UNK:O	1:L6:131:UNK:N	2.36	0.59
1:L1:211:UNK:O	1:L1:214:UNK:CB	2.51	0.58
1:L6:475:UNK:O	1:L6:479:UNK:CB	2.51	0.58
2:M6:42:UNK:O	2:M6:44:UNK:N	2.36	0.58
2:M3:356:UNK:O	2:M3:360:UNK:N	2.35	0.58
7:U3:22:UNK:O	7:U3:23:UNK:CB	2.52	0.58
1:L5:316:UNK:O	1:L5:319:UNK:CB	2.51	0.58
2:M5:42:UNK:O	2:M5:44:UNK:N	2.36	0.58
2:M5:324:UNK:O	2:M5:328:UNK:CB	2.50	0.58
1:L6:211:UNK:O	1:L6:214:UNK:CB	2.51	0.58
1:L2:475:UNK:O	1:L2:479:UNK:CB	2.51	0.58
2:M2:42:UNK:O	2:M2:44:UNK:N	2.36	0.58
10:t2:2:UNK:O	10:t2:3:UNK:C	2.52	0.58
1:L3:475:UNK:O	1:L3:479:UNK:CB	2.51	0.58
5:j3:14:UNK:O	5:j3:17:UNK:CB	2.51	0.58
1:L4:128:UNK:O	1:L4:131:UNK:N	2.36	0.58
2:M4:42:UNK:O	2:M4:44:UNK:N	2.36	0.58
10:t4:20:UNK:O	10:t4:21:UNK:CB	2.50	0.58
8:n5:5:UNK:O	8:n5:6:UNK:C	2.48	0.58
2:M6:75:UNK:O	2:M6:78:UNK:N	2.37	0.58
5:k6:23:UNK:O	5:k6:26:UNK:CB	2.51	0.58
2:M1:340:UNK:O	2:M1:342:UNK:N	2.37	0.58
5:k1:23:UNK:O	5:k1:26:UNK:CB	2.51	0.58
10:t1:9:UNK:O	10:t1:12:UNK:N	2.36	0.58
1:L2:382:UNK:CB	1:L2:389:UNK:HA	2.34	0.58
8:n2:50:UNK:O	8:n2:51:UNK:C	2.52	0.58
1:L4:211:UNK:O	1:L4:214:UNK:CB	2.51	0.58
2:M4:26:UNK:O	2:M4:27:UNK:C	2.47	0.58
1:L5:128:UNK:O	1:L5:131:UNK:N	2.36	0.58
2:M5:68:UNK:C	2:M5:70:UNK:N	2.66	0.58
2:M1:42:UNK:O	2:M1:44:UNK:N	2.36	0.58
3:i1:24:UNK:O	3:i1:27:UNK:CB	2.52	0.58
10:t1:20:UNK:O	10:t1:21:UNK:CB	2.50	0.58
8:n3:9:UNK:O	8:n3:12:UNK:CB	2.52	0.58
1:L5:382:UNK:CB	1:L5:389:UNK:HA	2.34	0.58
3:i5:24:UNK:O	3:i5:27:UNK:CB	2.52	0.58
5:k5:23:UNK:O	5:k5:26:UNK:CB	2.51	0.58
2:M6:108:UNK:CA	2:M6:111:UNK:CB	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M3:108:UNK:CA	2:M3:111:UNK:CB	2.81	0.58
7:U3:9:UNK:O	7:U3:12:UNK:CB	2.51	0.58
2:M4:75:UNK:O	2:M4:78:UNK:N	2.37	0.58
3:i4:24:UNK:O	3:i4:27:UNK:CB	2.52	0.58
8:n4:5:UNK:O	8:n4:6:UNK:C	2.48	0.58
10:t4:9:UNK:O	10:t4:12:UNK:N	2.36	0.58
14:BD:586:UNK:O	14:BD:587:UNK:C	2.51	0.58
8:n5:50:UNK:O	8:n5:51:UNK:C	2.52	0.58
10:t6:9:UNK:O	10:t6:12:UNK:N	2.36	0.58
3:i3:24:UNK:O	3:i3:27:UNK:CB	2.52	0.58
8:n4:50:UNK:O	8:n4:51:UNK:C	2.52	0.58
8:n6:9:UNK:O	8:n6:12:UNK:CB	2.52	0.58
1:L2:419:UNK:O	1:L2:422:UNK:N	2.37	0.58
14:BB:1614:UNK:C	14:BB:1617:UNK:CB	2.82	0.58
7:U3:23:UNK:CB	7:U3:24:UNK:CA	2.81	0.58
14:BC:1614:UNK:C	14:BC:1617:UNK:CB	2.82	0.58
14:BD:1614:UNK:C	14:BD:1617:UNK:N	2.65	0.58
2:M5:356:UNK:O	2:M5:360:UNK:N	2.35	0.58
1:L6:382:UNK:CB	1:L6:389:UNK:HA	2.34	0.58
1:L1:38:UNK:O	1:L1:41:UNK:N	2.37	0.58
1:L2:38:UNK:O	1:L2:41:UNK:N	2.37	0.58
1:L2:128:UNK:O	1:L2:131:UNK:N	2.36	0.58
14:BD:1614:UNK:C	14:BD:1617:UNK:CB	2.82	0.58
1:L5:38:UNK:O	1:L5:41:UNK:N	2.37	0.58
2:M5:75:UNK:O	2:M5:78:UNK:N	2.37	0.58
7:U5:9:UNK:O	7:U5:12:UNK:CB	2.51	0.58
14:BF:586:UNK:O	14:BF:587:UNK:C	2.51	0.58
1:L1:368:UNK:O	1:L1:372:UNK:N	2.37	0.58
1:L1:382:UNK:CB	1:L1:389:UNK:HA	2.34	0.58
1:L1:419:UNK:O	1:L1:422:UNK:N	2.37	0.58
8:n2:9:UNK:O	8:n2:12:UNK:CB	2.52	0.58
1:L4:368:UNK:O	1:L4:372:UNK:N	2.37	0.58
2:M4:340:UNK:O	2:M4:342:UNK:N	2.37	0.58
3:i6:24:UNK:O	3:i6:27:UNK:CB	2.52	0.58
14:BF:1614:UNK:C	14:BF:1617:UNK:CB	2.82	0.58
14:BB:586:UNK:O	14:BB:587:UNK:C	2.51	0.57
1:L6:116:UNK:O	1:L6:117:UNK:C	2.45	0.57
2:M1:75:UNK:O	2:M1:78:UNK:N	2.37	0.57
1:L2:368:UNK:O	1:L2:372:UNK:N	2.37	0.57
2:M2:340:UNK:O	2:M2:342:UNK:N	2.37	0.57
3:i2:24:UNK:O	3:i2:27:UNK:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L3:419:UNK:O	1:L3:422:UNK:N	2.37	0.57
2:M3:75:UNK:O	2:M3:78:UNK:N	2.37	0.57
1:L4:419:UNK:O	1:L4:422:UNK:N	2.37	0.57
1:L5:207:UNK:CA	1:L5:208:UNK:C	2.82	0.57
2:M5:293:UNK:O	2:M5:294:UNK:C	2.52	0.57
5:k1:17:UNK:O	5:k1:21:UNK:N	2.38	0.57
14:BA:1614:UNK:C	14:BA:1617:UNK:CB	2.82	0.57
1:L3:382:UNK:CB	1:L3:389:UNK:HA	2.34	0.57
10:t4:2:UNK:O	10:t4:3:UNK:C	2.52	0.57
1:L5:368:UNK:O	1:L5:372:UNK:N	2.37	0.57
2:M5:340:UNK:O	2:M5:342:UNK:N	2.37	0.57
14:BE:1614:UNK:C	14:BE:1617:UNK:CB	2.82	0.57
1:L6:207:UNK:CA	1:L6:208:UNK:C	2.82	0.57
2:M2:75:UNK:O	2:M2:78:UNK:N	2.37	0.57
2:M2:293:UNK:O	2:M2:294:UNK:C	2.52	0.57
2:M4:31:UNK:O	2:M4:32:UNK:O	2.23	0.57
7:U6:22:UNK:O	7:U6:23:UNK:CB	2.52	0.57
8:n1:50:UNK:O	8:n1:51:UNK:C	2.52	0.57
7:U2:22:UNK:O	7:U2:23:UNK:CB	2.52	0.57
10:t2:9:UNK:O	10:t2:12:UNK:N	2.36	0.57
14:BD:546:UNK:O	14:BE:1588:UNK:N	2.38	0.57
7:U5:23:UNK:CB	7:U5:24:UNK:CA	2.81	0.57
8:n1:9:UNK:O	8:n1:12:UNK:CB	2.52	0.57
5:k4:17:UNK:O	5:k4:21:UNK:N	2.38	0.57
1:L5:137:UNK:O	1:L5:140:UNK:N	2.38	0.57
10:t6:2:UNK:O	10:t6:3:UNK:C	2.52	0.57
2:M1:31:UNK:O	2:M1:32:UNK:O	2.23	0.57
7:U1:22:UNK:O	7:U1:23:UNK:CB	2.52	0.57
7:U1:23:UNK:CB	7:U1:24:UNK:CA	2.81	0.57
1:L2:137:UNK:O	1:L2:140:UNK:N	2.38	0.57
1:L2:207:UNK:CA	1:L2:208:UNK:C	2.82	0.57
1:L3:207:UNK:CA	1:L3:208:UNK:C	2.82	0.57
8:n3:50:UNK:O	8:n3:51:UNK:C	2.52	0.57
5:k5:17:UNK:O	5:k5:21:UNK:N	2.38	0.57
2:M6:410:UNK:O	2:M6:414:UNK:N	2.38	0.57
3:h1:6:UNK:O	3:h1:10:UNK:N	2.38	0.57
1:L3:137:UNK:O	1:L3:140:UNK:N	2.38	0.57
2:M4:293:UNK:O	2:M4:294:UNK:C	2.52	0.57
1:L5:419:UNK:O	1:L5:422:UNK:N	2.37	0.57
8:n5:9:UNK:O	8:n5:12:UNK:CB	2.52	0.57
1:L6:21:UNK:O	1:L6:22:UNK:C	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L6:368:UNK:O	1:L6:372:UNK:N	2.37	0.57
1:L1:207:UNK:CA	1:L1:208:UNK:C	2.82	0.57
1:L1:488:UNK:O	1:L1:489:UNK:C	2.50	0.57
2:M2:31:UNK:O	2:M2:32:UNK:O	2.23	0.57
1:L3:38:UNK:O	1:L3:41:UNK:N	2.37	0.57
8:n4:9:UNK:O	8:n4:12:UNK:CB	2.52	0.57
2:M5:91:UNK:O	2:M5:94:UNK:N	2.38	0.57
10:t5:2:UNK:O	10:t5:3:UNK:C	2.52	0.57
1:L6:38:UNK:O	1:L6:41:UNK:N	2.37	0.57
2:M6:340:UNK:O	2:M6:342:UNK:N	2.37	0.57
3:h6:6:UNK:O	3:h6:10:UNK:N	2.38	0.57
1:L1:65:UNK:CB	1:L1:66:UNK:CA	2.83	0.57
2:M2:91:UNK:O	2:M2:94:UNK:N	2.38	0.57
5:k2:17:UNK:O	5:k2:21:UNK:N	2.38	0.57
8:n2:45:UNK:O	8:n2:49:UNK:N	2.38	0.57
8:n3:45:UNK:O	8:n3:49:UNK:N	2.38	0.57
1:L4:137:UNK:O	1:L4:140:UNK:N	2.38	0.57
1:L4:382:UNK:CB	1:L4:389:UNK:HA	2.34	0.57
8:n6:45:UNK:O	8:n6:49:UNK:N	2.38	0.57
2:M1:121:UNK:O	2:M1:124:UNK:CB	2.53	0.56
4:g1:16:UNK:C	4:g1:18:UNK:N	2.67	0.56
10:t1:2:UNK:O	10:t1:3:UNK:C	2.52	0.56
1:L2:488:UNK:O	1:L2:489:UNK:C	2.50	0.56
1:L3:21:UNK:O	1:L3:22:UNK:C	2.52	0.56
10:t3:2:UNK:O	10:t3:3:UNK:C	2.52	0.56
3:h4:6:UNK:O	3:h4:10:UNK:N	2.38	0.56
1:L5:65:UNK:CB	1:L5:66:UNK:CA	2.83	0.56
2:M5:180:UNK:C	2:M5:182:UNK:N	2.65	0.56
3:h5:6:UNK:O	3:h5:10:UNK:N	2.38	0.56
1:L1:137:UNK:O	1:L1:140:UNK:N	2.38	0.56
2:M1:293:UNK:O	2:M1:294:UNK:C	2.52	0.56
8:n1:45:UNK:O	8:n1:49:UNK:N	2.38	0.56
2:M3:91:UNK:O	2:M3:94:UNK:N	2.38	0.56
2:M3:121:UNK:O	2:M3:124:UNK:CB	2.53	0.56
1:L4:38:UNK:O	1:L4:41:UNK:N	2.37	0.56
2:M4:42:UNK:O	2:M4:43:UNK:C	2.53	0.56
2:M4:121:UNK:O	2:M4:124:UNK:CB	2.53	0.56
2:M4:328:UNK:O	2:M4:329:UNK:C	2.52	0.56
1:L6:419:UNK:O	1:L6:422:UNK:N	2.37	0.56
1:L1:156:UNK:O	1:L1:157:UNK:CB	2.54	0.56
7:U1:10:UNK:O	7:U1:13:UNK:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:21:UNK:O	1:L2:22:UNK:C	2.52	0.56
1:L2:117:UNK:O	1:L2:118:UNK:C	2.54	0.56
1:L2:156:UNK:O	1:L2:157:UNK:CB	2.54	0.56
2:M2:410:UNK:O	2:M2:414:UNK:N	2.38	0.56
7:U2:10:UNK:O	7:U2:13:UNK:CB	2.54	0.56
1:L3:156:UNK:O	1:L3:157:UNK:CB	2.54	0.56
1:L3:351:UNK:O	1:L3:352:UNK:CB	2.53	0.56
3:h3:6:UNK:O	3:h3:10:UNK:N	2.38	0.56
1:L4:21:UNK:O	1:L4:22:UNK:C	2.53	0.56
1:L4:65:UNK:CB	1:L4:66:UNK:CA	2.83	0.56
1:L4:510:UNK:O	1:L4:513:UNK:CB	2.54	0.56
2:M4:68:UNK:C	2:M4:70:UNK:N	2.66	0.56
2:M4:410:UNK:O	2:M4:414:UNK:N	2.38	0.56
8:n4:45:UNK:O	8:n4:49:UNK:N	2.38	0.56
1:L5:21:UNK:O	1:L5:22:UNK:C	2.52	0.56
1:L5:376:UNK:C	1:L5:378:UNK:N	2.68	0.56
2:M5:31:UNK:O	2:M5:32:UNK:O	2.23	0.56
1:L6:65:UNK:CB	1:L6:66:UNK:CA	2.83	0.56
1:L6:510:UNK:O	1:L6:513:UNK:CB	2.54	0.56
8:n6:50:UNK:O	8:n6:51:UNK:C	2.52	0.56
1:L2:65:UNK:CB	1:L2:66:UNK:CA	2.83	0.56
2:M2:68:UNK:C	2:M2:70:UNK:N	2.66	0.56
5:k3:17:UNK:O	5:k3:21:UNK:N	2.38	0.56
14:BC:586:UNK:O	14:BC:587:UNK:C	2.51	0.56
7:U5:10:UNK:O	7:U5:13:UNK:CB	2.54	0.56
8:n5:45:UNK:O	8:n5:49:UNK:N	2.38	0.56
1:L1:47:UNK:O	1:L1:48:UNK:C	2.53	0.56
1:L1:366:UNK:O	1:L1:369:UNK:N	2.39	0.56
2:M1:42:UNK:O	2:M1:43:UNK:C	2.53	0.56
1:L3:368:UNK:O	1:L3:372:UNK:N	2.37	0.56
2:M3:42:UNK:O	2:M3:43:UNK:C	2.53	0.56
2:M3:340:UNK:O	2:M3:342:UNK:N	2.37	0.56
2:M3:410:UNK:O	2:M3:414:UNK:N	2.38	0.56
7:U3:49:UNK:O	7:U3:53:UNK:N	2.39	0.56
2:M4:91:UNK:O	2:M4:94:UNK:N	2.38	0.56
1:L6:156:UNK:O	1:L6:157:UNK:CB	2.54	0.56
2:M6:91:UNK:O	2:M6:94:UNK:N	2.38	0.56
2:M6:293:UNK:O	2:M6:294:UNK:C	2.52	0.56
2:M1:176:UNK:CB	2:M1:179:UNK:N	2.69	0.56
2:M2:94:UNK:O	2:M2:95:UNK:C	2.48	0.56
7:U2:49:UNK:O	7:U2:53:UNK:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L3:383:UNK:C	1:L3:389:UNK:CB	2.84	0.56
2:M6:31:UNK:O	2:M6:32:UNK:O	2.23	0.56
2:M1:91:UNK:O	2:M1:94:UNK:N	2.38	0.56
2:M1:328:UNK:O	2:M1:329:UNK:C	2.52	0.56
2:M2:42:UNK:O	2:M2:43:UNK:C	2.53	0.56
7:U4:23:UNK:CB	7:U4:24:UNK:CA	2.81	0.56
1:L5:512:UNK:O	1:L5:513:UNK:C	2.53	0.56
2:M5:410:UNK:O	2:M5:414:UNK:N	2.38	0.56
2:M6:176:UNK:CB	2:M6:179:UNK:N	2.69	0.56
4:g1:11:UNK:C	4:g1:13:UNK:N	2.69	0.56
1:L2:351:UNK:O	1:L2:352:UNK:CB	2.53	0.56
1:L2:366:UNK:O	1:L2:369:UNK:N	2.39	0.56
2:M2:121:UNK:O	2:M2:124:UNK:CB	2.53	0.56
2:M2:176:UNK:CB	2:M2:179:UNK:N	2.69	0.56
1:L3:512:UNK:O	1:L3:513:UNK:C	2.53	0.56
2:M3:31:UNK:O	2:M3:32:UNK:O	2.23	0.56
7:U4:49:UNK:O	7:U4:53:UNK:N	2.39	0.56
2:M5:176:UNK:CB	2:M5:179:UNK:N	2.69	0.56
4:g5:11:UNK:C	4:g5:13:UNK:N	2.69	0.56
14:BE:586:UNK:O	14:BE:587:UNK:C	2.51	0.56
2:M6:121:UNK:O	2:M6:124:UNK:CB	2.53	0.56
5:k6:17:UNK:O	5:k6:21:UNK:N	2.38	0.56
2:M1:410:UNK:O	2:M1:414:UNK:N	2.38	0.56
3:h2:6:UNK:O	3:h2:10:UNK:N	2.38	0.56
5:j2:10:UNK:O	5:j2:13:UNK:N	2.39	0.56
5:j3:10:UNK:O	5:j3:13:UNK:N	2.39	0.56
2:M4:176:UNK:CB	2:M4:179:UNK:N	2.69	0.56
7:U4:10:UNK:O	7:U4:13:UNK:CB	2.54	0.56
7:U5:49:UNK:O	7:U5:53:UNK:N	2.39	0.56
1:L6:351:UNK:O	1:L6:352:UNK:CB	2.53	0.56
1:L6:512:UNK:O	1:L6:513:UNK:C	2.53	0.56
1:L1:181:UNK:O	1:L1:183:UNK:N	2.39	0.56
1:L1:512:UNK:O	1:L1:513:UNK:C	2.53	0.56
1:L3:510:UNK:O	1:L3:513:UNK:CB	2.54	0.56
2:M3:94:UNK:O	2:M3:95:UNK:C	2.48	0.56
2:M3:293:UNK:O	2:M3:294:UNK:C	2.52	0.56
2:M4:94:UNK:O	2:M4:95:UNK:C	2.48	0.56
8:n4:10:UNK:C	8:n4:12:UNK:N	2.67	0.56
1:L5:510:UNK:O	1:L5:513:UNK:CB	2.54	0.56
2:M5:121:UNK:O	2:M5:124:UNK:CB	2.53	0.56
7:U6:10:UNK:O	7:U6:13:UNK:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:242:UNK:O	1:L1:245:UNK:N	2.39	0.55
7:U1:49:UNK:O	7:U1:53:UNK:N	2.39	0.55
1:L2:77:UNK:CA	1:L2:78:UNK:CB	2.84	0.55
1:L2:181:UNK:O	1:L2:183:UNK:N	2.39	0.55
1:L2:510:UNK:O	1:L2:513:UNK:CB	2.54	0.55
2:M3:176:UNK:CB	2:M3:179:UNK:N	2.69	0.55
1:L4:366:UNK:O	1:L4:369:UNK:N	2.39	0.55
1:L4:512:UNK:O	1:L4:513:UNK:C	2.53	0.55
1:L5:156:UNK:O	1:L5:157:UNK:CB	2.54	0.55
1:L5:207:UNK:CB	1:L5:208:UNK:C	2.84	0.55
1:L6:181:UNK:O	1:L6:183:UNK:N	2.39	0.55
5:j6:10:UNK:O	5:j6:13:UNK:N	2.39	0.55
1:L1:207:UNK:CB	1:L1:208:UNK:C	2.84	0.55
1:L1:351:UNK:O	1:L1:352:UNK:CB	2.53	0.55
1:L3:65:UNK:CB	1:L3:66:UNK:CA	2.83	0.55
1:L4:201:UNK:O	1:L4:202:UNK:C	2.54	0.55
1:L4:207:UNK:CB	1:L4:208:UNK:C	2.84	0.55
1:L4:383:UNK:C	1:L4:389:UNK:CB	2.84	0.55
1:L5:366:UNK:O	1:L5:369:UNK:N	2.39	0.55
1:L6:137:UNK:O	1:L6:140:UNK:N	2.38	0.55
1:L6:383:UNK:C	1:L6:389:UNK:CB	2.84	0.55
2:M6:227:UNK:CA	2:M6:228:UNK:CB	2.85	0.55
1:L1:21:UNK:O	1:L1:22:UNK:C	2.53	0.55
1:L1:383:UNK:C	1:L1:389:UNK:CB	2.84	0.55
2:M1:94:UNK:O	2:M1:97:UNK:N	2.40	0.55
2:M1:209:UNK:O	2:M1:211:UNK:O	2.25	0.55
1:L3:242:UNK:O	1:L3:245:UNK:N	2.39	0.55
5:j4:10:UNK:O	5:j4:13:UNK:N	2.39	0.55
14:BD:547:UNK:CB	14:BE:1590:UNK:CA	2.79	0.55
7:U5:22:UNK:O	7:U5:23:UNK:CB	2.52	0.55
1:L6:366:UNK:O	1:L6:369:UNK:N	2.39	0.55
10:t1:34:UNK:C	10:t1:36:UNK:N	2.68	0.55
1:L2:207:UNK:CB	1:L2:208:UNK:C	2.84	0.55
1:L2:383:UNK:C	1:L2:389:UNK:CB	2.84	0.55
2:M2:188:UNK:CB	2:M2:189:UNK:CB	2.85	0.55
1:L3:181:UNK:O	1:L3:183:UNK:N	2.39	0.55
2:M3:61:UNK:CA	2:M3:62:UNK:C	2.85	0.55
2:M4:227:UNK:CA	2:M4:228:UNK:CB	2.85	0.55
1:L5:65:UNK:CB	1:L5:66:UNK:C	2.83	0.55
1:L5:383:UNK:C	1:L5:389:UNK:CB	2.84	0.55
2:M6:94:UNK:O	2:M6:97:UNK:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:201:UNK:O	1:L1:202:UNK:C	2.54	0.55
1:L1:510:UNK:O	1:L1:513:UNK:CB	2.54	0.55
2:M1:94:UNK:O	2:M1:95:UNK:C	2.48	0.55
2:M1:188:UNK:CB	2:M1:189:UNK:CB	2.85	0.55
1:L2:242:UNK:O	1:L2:245:UNK:N	2.39	0.55
1:L2:512:UNK:O	1:L2:513:UNK:C	2.53	0.55
1:L3:201:UNK:O	1:L3:202:UNK:C	2.54	0.55
1:L3:366:UNK:O	1:L3:369:UNK:N	2.39	0.55
2:M3:209:UNK:O	2:M3:211:UNK:O	2.25	0.55
7:U3:30:UNK:CB	7:U3:34:UNK:CB	2.85	0.55
1:L4:156:UNK:O	1:L4:157:UNK:CB	2.54	0.55
2:M4:188:UNK:CB	2:M4:189:UNK:CB	2.85	0.55
2:M4:209:UNK:O	2:M4:211:UNK:O	2.25	0.55
3:i4:22:UNK:O	3:i4:23:UNK:C	2.54	0.55
1:L5:188:UNK:CB	1:L5:211:UNK:CB	2.84	0.55
1:L5:242:UNK:O	1:L5:245:UNK:N	2.39	0.55
2:M5:209:UNK:O	2:M5:211:UNK:O	2.25	0.55
1:L6:242:UNK:O	1:L6:245:UNK:N	2.39	0.55
2:M6:42:UNK:O	2:M6:43:UNK:C	2.53	0.55
2:M1:25:UNK:O	2:M1:26:UNK:C	2.55	0.55
5:j1:10:UNK:O	5:j1:13:UNK:N	2.39	0.55
7:U1:30:UNK:CB	7:U1:34:UNK:CB	2.85	0.55
1:L2:61:UNK:CB	1:L2:80:UNK:CB	2.85	0.55
1:L2:201:UNK:O	1:L2:202:UNK:C	2.54	0.55
2:M3:227:UNK:CA	2:M3:228:UNK:CB	2.85	0.55
1:L4:242:UNK:O	1:L4:245:UNK:N	2.39	0.55
7:U4:30:UNK:CB	7:U4:34:UNK:CB	2.85	0.55
2:M5:42:UNK:O	2:M5:43:UNK:C	2.53	0.55
2:M5:94:UNK:O	2:M5:97:UNK:N	2.40	0.55
7:U6:30:UNK:CB	7:U6:34:UNK:CB	2.85	0.55
7:U6:49:UNK:O	7:U6:53:UNK:N	2.39	0.55
1:L1:310:UNK:O	1:L1:313:UNK:CB	2.55	0.55
2:M2:227:UNK:CA	2:M2:228:UNK:CB	2.85	0.55
1:L3:188:UNK:CB	1:L3:211:UNK:CB	2.85	0.55
1:L3:310:UNK:O	1:L3:313:UNK:CB	2.55	0.55
1:L4:351:UNK:O	1:L4:352:UNK:CB	2.53	0.55
2:M4:94:UNK:O	2:M4:97:UNK:N	2.40	0.55
1:L5:111:UNK:CB	1:L5:114:UNK:CB	2.85	0.55
1:L5:181:UNK:O	1:L5:183:UNK:N	2.39	0.55
2:M5:188:UNK:CB	2:M5:189:UNK:CB	2.85	0.55
3:i5:22:UNK:O	3:i5:23:UNK:C	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j5:10:UNK:O	5:j5:13:UNK:N	2.39	0.55
1:L6:188:UNK:CB	1:L6:211:UNK:CB	2.85	0.55
1:L6:207:UNK:CB	1:L6:208:UNK:C	2.84	0.55
2:M6:209:UNK:O	2:M6:211:UNK:O	2.25	0.55
1:L1:376:UNK:C	1:L1:378:UNK:N	2.68	0.55
1:L2:28:UNK:CB	1:L2:31:UNK:CB	2.85	0.55
2:M2:133:UNK:CA	2:M2:224:UNK:CB	2.85	0.55
1:L3:117:UNK:O	1:L3:118:UNK:C	2.54	0.55
2:M3:279:UNK:CB	2:M3:280:UNK:CA	2.85	0.55
7:U3:10:UNK:O	7:U3:13:UNK:CB	2.54	0.55
1:L4:188:UNK:CB	1:L4:211:UNK:CB	2.85	0.55
2:M4:61:UNK:CA	2:M4:62:UNK:C	2.85	0.55
1:L5:117:UNK:O	1:L5:118:UNK:C	2.54	0.55
1:L5:201:UNK:O	1:L5:202:UNK:C	2.54	0.55
1:L5:351:UNK:O	1:L5:352:UNK:CB	2.53	0.55
1:L6:197:UNK:CB	1:L6:200:UNK:CB	2.85	0.55
2:M6:113:UNK:CA	2:M6:114:UNK:C	2.85	0.55
1:L2:38:UNK:O	1:L2:39:UNK:C	2.55	0.55
2:M2:372:UNK:CB	2:M2:375:UNK:CB	2.85	0.55
1:L3:197:UNK:CB	1:L3:200:UNK:CB	2.85	0.55
14:BD:1637:UNK:HA	14:BD:1639:UNK:O	2.07	0.55
1:L5:310:UNK:O	1:L5:313:UNK:CB	2.55	0.55
2:M5:227:UNK:CA	2:M5:228:UNK:CB	2.85	0.55
1:L6:310:UNK:O	1:L6:313:UNK:CB	2.55	0.55
2:M6:94:UNK:O	2:M6:95:UNK:C	2.48	0.55
1:L1:117:UNK:O	1:L1:118:UNK:C	2.54	0.55
1:L1:188:UNK:CB	1:L1:211:UNK:CB	2.85	0.55
2:M1:61:UNK:CA	2:M1:62:UNK:C	2.85	0.55
7:U1:43:UNK:CB	7:U1:46:UNK:CB	2.85	0.55
4:g2:16:UNK:C	4:g2:18:UNK:N	2.67	0.55
1:L4:197:UNK:CB	1:L4:200:UNK:CB	2.85	0.55
2:M4:176:UNK:O	5:s4:18:UNK:CB	2.56	0.55
8:n1:10:UNK:C	8:n1:12:UNK:N	2.67	0.54
1:L2:197:UNK:CB	1:L2:200:UNK:CB	2.85	0.54
2:M2:176:UNK:O	5:s2:18:UNK:CB	2.56	0.54
2:M2:241:UNK:O	2:M2:243:UNK:N	2.40	0.54
7:U2:30:UNK:CB	7:U2:34:UNK:CB	2.85	0.54
1:L3:207:UNK:CB	1:L3:208:UNK:C	2.84	0.54
2:M3:188:UNK:CB	2:M3:189:UNK:CB	2.85	0.54
4:g3:11:UNK:C	4:g3:13:UNK:N	2.69	0.54
1:L4:55:UNK:CB	1:L4:56:UNK:CB	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M4:372:UNK:CB	2:M4:375:UNK:CB	2.85	0.54
7:U4:43:UNK:CB	7:U4:46:UNK:CB	2.85	0.54
2:M5:372:UNK:CB	2:M5:375:UNK:CB	2.85	0.54
14:BE:1637:UNK:HA	14:BE:1639:UNK:O	2.08	0.54
1:L6:38:UNK:O	1:L6:39:UNK:C	2.55	0.54
1:L6:176:UNK:O	1:L6:179:UNK:CB	2.56	0.54
4:g6:16:UNK:C	4:g6:18:UNK:N	2.67	0.54
7:U6:43:UNK:CB	7:U6:46:UNK:CB	2.85	0.54
14:BF:1637:UNK:HA	14:BF:1639:UNK:O	2.07	0.54
1:L1:55:UNK:CB	1:L1:56:UNK:CB	2.86	0.54
1:L1:176:UNK:O	1:L1:179:UNK:CB	2.56	0.54
2:M1:227:UNK:CA	2:M1:228:UNK:CB	2.85	0.54
1:L2:188:UNK:CB	1:L2:211:UNK:CB	2.84	0.54
1:L2:210:UNK:O	1:L2:213:UNK:N	2.41	0.54
2:M3:241:UNK:O	2:M3:243:UNK:N	2.40	0.54
7:U3:43:UNK:CB	7:U3:46:UNK:CB	2.85	0.54
7:U4:22:UNK:O	7:U4:23:UNK:CB	2.52	0.54
1:L5:55:UNK:CB	1:L5:56:UNK:CB	2.85	0.54
1:L5:210:UNK:O	1:L5:213:UNK:N	2.41	0.54
2:M5:61:UNK:CA	2:M5:62:UNK:C	2.85	0.54
2:M6:241:UNK:O	2:M6:243:UNK:N	2.40	0.54
3:i6:22:UNK:O	3:i6:23:UNK:C	2.54	0.54
1:L1:61:UNK:CB	1:L1:80:UNK:CB	2.85	0.54
3:i1:1:UNK:O	3:i1:2:UNK:C	2.56	0.54
14:BA:586:UNK:O	14:BA:587:UNK:C	2.51	0.54
14:BA:1637:UNK:HA	14:BA:1639:UNK:O	2.08	0.54
2:M2:328:UNK:O	2:M2:329:UNK:C	2.52	0.54
1:L3:28:UNK:CB	1:L3:31:UNK:CB	2.85	0.54
1:L3:61:UNK:CB	1:L3:80:UNK:CB	2.85	0.54
2:M3:68:UNK:C	2:M3:70:UNK:N	2.66	0.54
2:M3:176:UNK:O	5:s3:18:UNK:CB	2.55	0.54
3:i3:22:UNK:O	3:i3:23:UNK:C	2.54	0.54
1:L4:28:UNK:CB	1:L4:31:UNK:CB	2.85	0.54
1:L4:176:UNK:O	1:L4:179:UNK:CB	2.56	0.54
2:M5:113:UNK:CA	2:M5:114:UNK:C	2.85	0.54
3:i5:1:UNK:O	3:i5:2:UNK:C	2.56	0.54
1:L6:117:UNK:O	1:L6:118:UNK:C	2.54	0.54
1:L2:55:UNK:CB	1:L2:56:UNK:CB	2.85	0.54
2:M2:94:UNK:O	2:M2:97:UNK:N	2.40	0.54
7:U2:43:UNK:CB	7:U2:46:UNK:CB	2.85	0.54
1:L3:38:UNK:O	1:L3:39:UNK:C	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L3:111:UNK:CB	1:L3:114:UNK:CB	2.85	0.54
1:L3:176:UNK:O	1:L3:179:UNK:CB	2.56	0.54
1:L4:61:UNK:CB	1:L4:80:UNK:CB	2.85	0.54
1:L4:111:UNK:CB	1:L4:114:UNK:CB	2.85	0.54
1:L4:181:UNK:O	1:L4:183:UNK:N	2.39	0.54
1:L4:310:UNK:O	1:L4:313:UNK:CB	2.55	0.54
2:M4:113:UNK:CA	2:M4:114:UNK:C	2.85	0.54
2:M4:241:UNK:O	2:M4:243:UNK:N	2.40	0.54
2:M6:133:UNK:CA	2:M6:224:UNK:CB	2.85	0.54
1:L1:197:UNK:CB	1:L1:200:UNK:CB	2.85	0.54
1:L1:210:UNK:O	1:L1:213:UNK:N	2.41	0.54
2:M1:372:UNK:CB	2:M1:375:UNK:CB	2.85	0.54
8:n5:44:UNK:O	8:n5:45:UNK:C	2.55	0.54
2:M6:61:UNK:CA	2:M6:62:UNK:C	2.85	0.54
2:M6:188:UNK:CB	2:M6:189:UNK:CB	2.85	0.54
2:M6:279:UNK:CB	2:M6:280:UNK:CA	2.85	0.54
1:L1:111:UNK:CB	1:L1:114:UNK:CB	2.85	0.54
3:i2:22:UNK:O	3:i2:23:UNK:C	2.54	0.54
14:BB:1637:UNK:HA	14:BB:1639:UNK:O	2.07	0.54
1:L3:210:UNK:O	1:L3:213:UNK:N	2.41	0.54
2:M3:113:UNK:CA	2:M3:114:UNK:C	2.85	0.54
14:BC:1637:UNK:HA	14:BC:1639:UNK:O	2.07	0.54
1:L5:127:UNK:O	1:L5:131:UNK:N	2.41	0.54
8:n5:10:UNK:C	8:n5:12:UNK:N	2.67	0.54
1:L6:111:UNK:CB	1:L6:114:UNK:CB	2.85	0.54
2:M1:133:UNK:CA	2:M1:224:UNK:CB	2.85	0.54
1:L2:111:UNK:CB	1:L2:114:UNK:CB	2.85	0.54
1:L3:488:UNK:O	1:L3:489:UNK:C	2.50	0.54
1:L4:207:UNK:CA	1:L4:208:UNK:C	2.82	0.54
2:M4:279:UNK:CB	2:M4:280:UNK:CA	2.85	0.54
2:M4:343:UNK:C	2:M4:345:UNK:N	2.71	0.54
1:L5:61:UNK:CB	1:L5:80:UNK:CB	2.85	0.54
1:L5:176:UNK:O	1:L5:179:UNK:CB	2.56	0.54
1:L6:55:UNK:CB	1:L6:56:UNK:CB	2.86	0.54
1:L2:127:UNK:O	1:L2:131:UNK:N	2.41	0.54
2:M2:343:UNK:C	2:M2:345:UNK:N	2.71	0.54
4:g2:11:UNK:C	4:g2:13:UNK:N	2.69	0.54
1:L3:69:UNK:CB	1:L3:74:UNK:HA	2.38	0.54
1:L3:127:UNK:O	1:L3:131:UNK:N	2.41	0.54
2:M3:372:UNK:CB	2:M3:375:UNK:CB	2.85	0.54
4:g3:16:UNK:C	4:g3:18:UNK:N	2.67	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M4:180:UNK:C	2:M4:182:UNK:N	2.65	0.54
1:L5:28:UNK:CB	1:L5:31:UNK:CB	2.85	0.54
7:U5:30:UNK:CB	7:U5:34:UNK:CB	2.85	0.54
5:s5:14:UNK:O	5:s5:18:UNK:N	2.41	0.54
14:BE:1600:UNK:O	14:BE:1604:UNK:CB	2.56	0.54
1:L1:28:UNK:CB	1:L1:31:UNK:CB	2.85	0.54
1:L1:38:UNK:O	1:L1:39:UNK:C	2.55	0.54
1:L1:69:UNK:CB	1:L1:74:UNK:HA	2.38	0.54
2:M1:176:UNK:O	5:s1:18:UNK:CB	2.55	0.54
1:L2:176:UNK:O	1:L2:179:UNK:CB	2.56	0.54
2:M2:391:UNK:O	2:M2:392:UNK:CB	2.56	0.54
1:L3:55:UNK:CB	1:L3:56:UNK:CB	2.86	0.54
2:M3:25:UNK:O	2:M3:26:UNK:C	2.55	0.54
2:M3:180:UNK:C	2:M3:182:UNK:N	2.65	0.54
1:L5:47:UNK:O	1:L5:48:UNK:C	2.53	0.54
2:M5:25:UNK:O	2:M5:26:UNK:C	2.55	0.54
2:M5:133:UNK:CA	2:M5:224:UNK:CB	2.85	0.54
2:M5:343:UNK:C	2:M5:345:UNK:N	2.71	0.54
1:L6:61:UNK:CB	1:L6:80:UNK:CB	2.85	0.54
2:M1:325:UNK:O	2:M1:329:UNK:N	2.42	0.54
1:L4:31:UNK:O	1:L4:35:UNK:N	2.41	0.54
1:L4:47:UNK:O	1:L4:48:UNK:C	2.53	0.54
3:i4:1:UNK:O	3:i4:2:UNK:C	2.56	0.54
5:s4:14:UNK:O	5:s4:18:UNK:N	2.41	0.54
1:L5:197:UNK:CB	1:L5:200:UNK:CB	2.85	0.54
1:L6:31:UNK:O	1:L6:35:UNK:N	2.41	0.54
10:t6:34:UNK:C	10:t6:36:UNK:N	2.68	0.54
1:L1:77:UNK:CA	1:L1:78:UNK:CB	2.84	0.53
1:L2:31:UNK:O	1:L2:35:UNK:N	2.41	0.53
2:M2:209:UNK:O	2:M2:211:UNK:O	2.25	0.53
2:M2:279:UNK:CB	2:M2:280:UNK:CA	2.85	0.53
2:M2:325:UNK:O	2:M2:329:UNK:N	2.41	0.53
3:i2:1:UNK:O	3:i2:2:UNK:C	2.56	0.53
2:M3:133:UNK:CA	2:M3:224:UNK:CB	2.85	0.53
2:M3:325:UNK:O	2:M3:329:UNK:N	2.42	0.53
10:t3:2:UNK:O	10:t3:5:UNK:CB	2.56	0.53
14:BC:1600:UNK:O	14:BC:1604:UNK:CB	2.56	0.53
1:L4:210:UNK:O	1:L4:213:UNK:N	2.41	0.53
1:L5:69:UNK:CB	1:L5:74:UNK:HA	2.38	0.53
1:L6:55:UNK:N	1:L6:56:UNK:C	2.71	0.53
1:L6:376:UNK:C	1:L6:378:UNK:N	2.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M6:325:UNK:O	2:M6:329:UNK:N	2.42	0.53
8:n6:10:UNK:C	8:n6:12:UNK:N	2.67	0.53
1:L1:55:UNK:N	1:L1:56:UNK:C	2.71	0.53
1:L1:127:UNK:O	1:L1:131:UNK:N	2.41	0.53
1:L2:310:UNK:O	1:L2:313:UNK:CB	2.55	0.53
2:M2:61:UNK:CA	2:M2:62:UNK:C	2.85	0.53
2:M2:364:UNK:O	2:M2:367:UNK:CB	2.56	0.53
10:t2:2:UNK:O	10:t2:5:UNK:CB	2.56	0.53
1:L3:55:UNK:N	1:L3:56:UNK:C	2.71	0.53
5:s3:14:UNK:O	5:s3:18:UNK:N	2.41	0.53
1:L5:31:UNK:O	1:L5:35:UNK:N	2.41	0.53
2:M5:362:UNK:O	2:M5:365:UNK:N	2.42	0.53
1:L6:28:UNK:CB	1:L6:31:UNK:CB	2.85	0.53
1:L6:210:UNK:O	1:L6:213:UNK:N	2.41	0.53
2:M6:362:UNK:O	2:M6:365:UNK:N	2.42	0.53
2:M6:372:UNK:CB	2:M6:375:UNK:CB	2.85	0.53
5:s6:14:UNK:O	5:s6:18:UNK:N	2.41	0.53
2:M1:391:UNK:O	2:M1:392:UNK:CB	2.56	0.53
3:i1:22:UNK:O	3:i1:23:UNK:C	2.54	0.53
10:t1:2:UNK:O	10:t1:5:UNK:CB	2.56	0.53
2:M2:25:UNK:O	2:M2:26:UNK:C	2.55	0.53
1:L3:376:UNK:C	1:L3:378:UNK:N	2.68	0.53
2:M3:94:UNK:O	2:M3:97:UNK:N	2.40	0.53
2:M3:362:UNK:O	2:M3:365:UNK:N	2.42	0.53
2:M3:364:UNK:O	2:M3:367:UNK:CB	2.56	0.53
1:L4:376:UNK:C	1:L4:378:UNK:N	2.68	0.53
1:L5:38:UNK:O	1:L5:39:UNK:C	2.55	0.53
1:L6:47:UNK:O	1:L6:48:UNK:C	2.53	0.53
1:L6:69:UNK:CB	1:L6:74:UNK:HA	2.38	0.53
2:M6:176:UNK:O	5:s6:18:UNK:CB	2.56	0.53
1:L1:31:UNK:O	1:L1:35:UNK:N	2.41	0.53
2:M1:180:UNK:C	2:M1:182:UNK:N	2.65	0.53
2:M1:241:UNK:O	2:M1:243:UNK:N	2.40	0.53
2:M1:364:UNK:O	2:M1:367:UNK:N	2.42	0.53
13:w1:26:UNK:O	13:w1:27:UNK:C	2.57	0.53
1:L2:69:UNK:CB	1:L2:74:UNK:HA	2.38	0.53
5:s2:14:UNK:O	5:s2:18:UNK:N	2.41	0.53
1:L3:31:UNK:O	1:L3:35:UNK:N	2.41	0.53
2:M3:393:UNK:O	2:M3:394:UNK:C	2.56	0.53
1:L4:69:UNK:CB	1:L4:74:UNK:HA	2.38	0.53
1:L4:117:UNK:O	1:L4:118:UNK:C	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:127:UNK:O	1:L4:131:UNK:N	2.41	0.53
2:M4:133:UNK:CA	2:M4:224:UNK:CB	2.85	0.53
13:w4:26:UNK:O	13:w4:27:UNK:C	2.57	0.53
14:BD:547:UNK:C	14:BE:1591:UNK:N	2.70	0.53
2:M5:241:UNK:O	2:M5:243:UNK:N	2.40	0.53
2:M5:364:UNK:O	2:M5:367:UNK:N	2.42	0.53
3:f5:17:UNK:O	3:f5:21:UNK:N	2.42	0.53
7:U5:43:UNK:CB	7:U5:46:UNK:CB	2.85	0.53
2:M6:343:UNK:C	2:M6:345:UNK:N	2.71	0.53
10:t6:2:UNK:O	10:t6:5:UNK:CB	2.56	0.53
2:M1:279:UNK:CB	2:M1:280:UNK:CA	2.85	0.53
5:s1:14:UNK:O	5:s1:18:UNK:N	2.41	0.53
8:n2:44:UNK:O	8:n2:45:UNK:C	2.56	0.53
1:L5:77:UNK:CA	1:L5:78:UNK:CB	2.84	0.53
2:M5:176:UNK:O	5:s5:18:UNK:CB	2.55	0.53
2:M5:341:UNK:O	2:M5:342:UNK:C	2.56	0.53
2:M5:393:UNK:O	2:M5:394:UNK:C	2.57	0.53
10:t5:2:UNK:O	10:t5:5:UNK:CB	2.56	0.53
2:M6:391:UNK:O	2:M6:392:UNK:CB	2.56	0.53
14:BF:1600:UNK:O	14:BF:1604:UNK:CB	2.56	0.53
2:M1:227:UNK:N	2:M1:228:UNK:CB	2.72	0.53
2:M1:341:UNK:O	2:M1:342:UNK:C	2.56	0.53
2:M1:362:UNK:O	2:M1:365:UNK:N	2.42	0.53
2:M2:180:UNK:C	2:M2:182:UNK:N	2.65	0.53
2:M2:341:UNK:O	2:M2:342:UNK:C	2.56	0.53
1:L4:55:UNK:N	1:L4:56:UNK:C	2.71	0.53
1:L4:94:UNK:O	1:L4:95:UNK:C	2.56	0.53
1:L4:488:UNK:O	1:L4:489:UNK:C	2.50	0.53
2:M4:364:UNK:O	2:M4:367:UNK:CB	2.56	0.53
14:BD:1600:UNK:O	14:BD:1604:UNK:CB	2.56	0.53
1:L6:127:UNK:O	1:L6:131:UNK:N	2.41	0.53
2:M6:25:UNK:O	2:M6:26:UNK:C	2.55	0.53
2:M6:256:UNK:O	2:M6:257:UNK:C	2.56	0.53
7:U6:23:UNK:CB	7:U6:24:UNK:CA	2.81	0.53
2:M1:256:UNK:O	2:M1:257:UNK:C	2.56	0.53
2:M1:393:UNK:O	2:M1:394:UNK:C	2.57	0.53
1:L2:383:UNK:N	1:L2:389:UNK:CB	2.72	0.53
2:M2:241:UNK:C	2:M2:243:UNK:N	2.71	0.53
13:w2:26:UNK:O	13:w2:27:UNK:C	2.57	0.53
2:M3:3:UNK:H	2:M3:6:UNK:CB	2.22	0.53
2:M3:364:UNK:O	2:M3:367:UNK:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f3:17:UNK:O	3:f3:21:UNK:N	2.42	0.53
2:M4:391:UNK:O	2:M4:392:UNK:CB	2.56	0.53
8:n4:44:UNK:O	8:n4:45:UNK:C	2.55	0.53
1:L5:55:UNK:N	1:L5:56:UNK:C	2.71	0.53
1:L5:67:UNK:CB	1:L5:75:UNK:O	2.57	0.53
1:L6:67:UNK:CB	1:L6:75:UNK:O	2.57	0.53
2:M1:364:UNK:O	2:M1:367:UNK:CB	2.56	0.53
1:L2:181:UNK:C	1:L2:183:UNK:N	2.71	0.53
14:BB:1600:UNK:O	14:BB:1604:UNK:CB	2.56	0.53
2:M3:341:UNK:O	2:M3:342:UNK:C	2.56	0.53
2:M4:241:UNK:C	2:M4:243:UNK:N	2.71	0.53
2:M4:325:UNK:O	2:M4:329:UNK:N	2.41	0.53
7:U4:37:UNK:HA	7:U4:42:UNK:CB	2.39	0.53
10:t4:2:UNK:O	10:t4:5:UNK:CB	2.56	0.53
2:M6:392:UNK:C	2:M6:394:UNK:N	2.68	0.53
3:f6:17:UNK:O	3:f6:21:UNK:N	2.42	0.53
1:L1:67:UNK:CB	1:L1:75:UNK:O	2.57	0.53
2:M2:227:UNK:N	2:M2:228:UNK:CB	2.72	0.53
2:M2:364:UNK:O	2:M2:367:UNK:N	2.42	0.53
7:U2:37:UNK:HA	7:U2:42:UNK:CB	2.39	0.53
8:n2:25:UNK:O	8:n2:28:UNK:N	2.42	0.53
3:i3:1:UNK:O	3:i3:2:UNK:C	2.56	0.53
13:w3:26:UNK:O	13:w3:27:UNK:C	2.57	0.53
1:L4:38:UNK:O	1:L4:39:UNK:C	2.55	0.53
2:M4:341:UNK:O	2:M4:342:UNK:C	2.56	0.53
2:M5:325:UNK:O	2:M5:329:UNK:N	2.42	0.53
1:L6:383:UNK:N	1:L6:389:UNK:CB	2.72	0.53
2:M6:341:UNK:O	2:M6:342:UNK:C	2.56	0.53
3:i6:1:UNK:O	3:i6:2:UNK:C	2.56	0.53
1:L2:67:UNK:CB	1:L2:75:UNK:O	2.57	0.53
1:L2:241:UNK:O	1:L2:244:UNK:CB	2.57	0.53
1:L3:181:UNK:C	1:L3:183:UNK:N	2.71	0.53
1:L4:241:UNK:O	1:L4:244:UNK:CB	2.57	0.53
2:M4:362:UNK:O	2:M4:365:UNK:N	2.42	0.53
2:M5:279:UNK:CB	2:M5:280:UNK:CA	2.85	0.53
1:L6:207:UNK:CB	1:L6:209:UNK:N	2.72	0.53
2:M6:227:UNK:N	2:M6:228:UNK:CB	2.72	0.53
2:M6:364:UNK:O	2:M6:367:UNK:N	2.42	0.53
14:BA:1600:UNK:O	14:BA:1604:UNK:CB	2.56	0.52
1:L2:47:UNK:O	1:L2:48:UNK:C	2.53	0.52
1:L2:94:UNK:O	1:L2:95:UNK:C	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:161:UNK:CB	1:L2:162:UNK:HA	2.40	0.52
1:L2:207:UNK:CB	1:L2:209:UNK:N	2.72	0.52
2:M2:362:UNK:O	2:M2:365:UNK:N	2.42	0.52
3:f2:17:UNK:O	3:f2:21:UNK:N	2.42	0.52
1:L3:383:UNK:N	1:L3:389:UNK:CB	2.72	0.52
2:M3:227:UNK:N	2:M3:228:UNK:CB	2.72	0.52
7:U3:37:UNK:HA	7:U3:42:UNK:CB	2.39	0.52
1:L4:161:UNK:HA	1:L4:163:UNK:CA	2.38	0.52
2:M4:287:UNK:O	2:M4:288:UNK:C	2.57	0.52
2:M5:328:UNK:O	2:M5:329:UNK:C	2.52	0.52
1:L6:161:UNK:CB	1:L6:162:UNK:HA	2.40	0.52
8:n6:25:UNK:O	8:n6:28:UNK:N	2.42	0.52
12:v6:21:UNK:O	12:v6:25:UNK:N	2.42	0.52
1:L1:207:UNK:CB	1:L1:209:UNK:N	2.72	0.52
7:U1:37:UNK:HA	7:U1:42:UNK:CB	2.39	0.52
11:u2:5:UNK:O	11:u2:8:UNK:N	2.43	0.52
1:L3:323:UNK:CB	1:L3:475:UNK:CB	2.88	0.52
1:L4:67:UNK:CB	1:L4:75:UNK:O	2.57	0.52
2:M4:364:UNK:O	2:M4:367:UNK:N	2.42	0.52
1:L5:94:UNK:O	1:L5:95:UNK:C	2.56	0.52
13:w5:3:UNK:O	13:w5:4:UNK:C	2.56	0.52
2:M6:61:UNK:N	2:M6:62:UNK:C	2.73	0.52
2:M6:364:UNK:O	2:M6:367:UNK:CB	2.56	0.52
2:M1:61:UNK:N	2:M1:62:UNK:C	2.73	0.52
2:M1:68:UNK:C	2:M1:70:UNK:N	2.66	0.52
12:v1:21:UNK:O	12:v1:25:UNK:N	2.42	0.52
1:L3:65:UNK:CB	1:L3:66:UNK:C	2.83	0.52
11:u3:5:UNK:O	11:u3:8:UNK:N	2.43	0.52
1:L4:383:UNK:N	1:L4:389:UNK:CB	2.72	0.52
2:M4:256:UNK:O	2:M4:257:UNK:C	2.56	0.52
13:w4:3:UNK:O	13:w4:4:UNK:C	2.56	0.52
2:M5:227:UNK:N	2:M5:228:UNK:CB	2.72	0.52
2:M5:364:UNK:O	2:M5:367:UNK:CB	2.56	0.52
1:L6:201:UNK:O	1:L6:202:UNK:C	2.54	0.52
2:M2:393:UNK:O	2:M2:394:UNK:C	2.57	0.52
1:L3:207:UNK:CB	1:L3:209:UNK:N	2.72	0.52
2:M3:287:UNK:O	2:M3:288:UNK:C	2.57	0.52
1:L4:323:UNK:CB	1:L4:475:UNK:CB	2.88	0.52
2:M4:25:UNK:O	2:M4:26:UNK:C	2.55	0.52
4:g4:11:UNK:C	4:g4:13:UNK:N	2.69	0.52
1:L5:207:UNK:CB	1:L5:209:UNK:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M5:114:UNK:N	2:M5:177:UNK:CB	2.73	0.52
2:M5:241:UNK:C	2:M5:243:UNK:N	2.71	0.52
11:u5:5:UNK:O	11:u5:8:UNK:N	2.43	0.52
1:L6:241:UNK:O	1:L6:244:UNK:CB	2.57	0.52
2:M6:3:UNK:H	2:M6:6:UNK:CB	2.22	0.52
2:M6:393:UNK:O	2:M6:394:UNK:C	2.57	0.52
3:f1:17:UNK:O	3:f1:21:UNK:N	2.42	0.52
1:L2:376:UNK:C	1:L2:378:UNK:N	2.68	0.52
2:M2:114:UNK:N	2:M2:177:UNK:CB	2.72	0.52
2:M2:115:UNK:N	2:M2:175:UNK:CB	2.73	0.52
2:M3:114:UNK:N	2:M3:177:UNK:CB	2.72	0.52
8:n3:25:UNK:O	8:n3:28:UNK:N	2.42	0.52
3:f4:17:UNK:O	3:f4:21:UNK:N	2.42	0.52
1:L6:279:UNK:O	1:L6:282:UNK:N	2.43	0.52
1:L6:323:UNK:CB	1:L6:475:UNK:CB	2.88	0.52
3:i6:22:UNK:C	3:i6:24:UNK:N	2.71	0.52
2:M2:113:UNK:CA	2:M2:114:UNK:C	2.85	0.52
1:L3:67:UNK:CB	1:L3:75:UNK:O	2.57	0.52
1:L3:161:UNK:CB	1:L3:162:UNK:HA	2.40	0.52
1:L3:241:UNK:O	1:L3:244:UNK:CB	2.57	0.52
1:L3:279:UNK:O	1:L3:282:UNK:N	2.43	0.52
2:M3:256:UNK:O	2:M3:257:UNK:C	2.56	0.52
3:i3:22:UNK:C	3:i3:24:UNK:N	2.71	0.52
14:BC:1588:UNK:N	14:BF:547:UNK:C	2.71	0.52
1:L4:279:UNK:O	1:L4:282:UNK:N	2.43	0.52
2:M4:61:UNK:N	2:M4:62:UNK:C	2.73	0.52
2:M4:309:UNK:O	2:M4:312:UNK:N	2.43	0.52
2:M5:27:UNK:O	2:M5:28:UNK:C	2.58	0.52
1:L6:488:UNK:O	1:L6:489:UNK:C	2.50	0.52
2:M6:62:UNK:CB	2:M6:64:UNK:N	2.73	0.52
2:M6:309:UNK:O	2:M6:312:UNK:N	2.43	0.52
4:g6:11:UNK:C	4:g6:13:UNK:N	2.69	0.52
1:L1:82:UNK:N	1:L1:86:UNK:CB	2.73	0.52
1:L1:323:UNK:CB	1:L1:475:UNK:CB	2.88	0.52
2:M1:139:UNK:HA	2:M1:140:UNK:CB	2.39	0.52
2:M1:190:UNK:N	2:M1:191:UNK:C	2.73	0.52
1:L2:82:UNK:N	1:L2:86:UNK:CB	2.73	0.52
2:M2:62:UNK:CB	2:M2:64:UNK:N	2.73	0.52
7:U2:23:UNK:CB	7:U2:24:UNK:CA	2.81	0.52
12:v2:21:UNK:O	12:v2:25:UNK:N	2.42	0.52
1:L3:82:UNK:N	1:L3:86:UNK:CB	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M3:391:UNK:O	2:M3:392:UNK:CB	2.56	0.52
8:n3:10:UNK:C	8:n3:12:UNK:N	2.67	0.52
1:L4:207:UNK:CB	1:L4:209:UNK:N	2.72	0.52
1:L5:82:UNK:N	1:L5:86:UNK:CB	2.73	0.52
1:L5:163:UNK:C	1:L5:165:UNK:N	2.69	0.52
2:M5:287:UNK:O	2:M5:288:UNK:C	2.57	0.52
2:M5:347:UNK:HA	2:M5:415:UNK:HA	1.92	0.52
2:M5:378:UNK:C	2:M5:380:UNK:N	2.72	0.52
7:U5:37:UNK:HA	7:U5:42:UNK:CB	2.39	0.52
10:t5:34:UNK:C	10:t5:36:UNK:N	2.68	0.52
13:w6:3:UNK:O	13:w6:4:UNK:C	2.56	0.52
1:L1:279:UNK:O	1:L1:282:UNK:N	2.43	0.52
1:L1:383:UNK:N	1:L1:389:UNK:CB	2.72	0.52
2:M1:287:UNK:O	2:M1:288:UNK:C	2.57	0.52
8:n1:25:UNK:O	8:n1:28:UNK:N	2.42	0.52
1:L2:323:UNK:CB	1:L2:475:UNK:CB	2.88	0.52
10:t2:34:UNK:C	10:t2:36:UNK:N	2.68	0.52
1:L4:161:UNK:CB	1:L4:162:UNK:HA	2.40	0.52
11:u4:5:UNK:O	11:u4:8:UNK:N	2.42	0.52
1:L5:161:UNK:CB	1:L5:162:UNK:HA	2.40	0.52
1:L5:241:UNK:O	1:L5:244:UNK:CB	2.57	0.52
1:L5:279:UNK:O	1:L5:282:UNK:N	2.43	0.52
1:L5:383:UNK:N	1:L5:389:UNK:CB	2.72	0.52
1:L5:488:UNK:O	1:L5:489:UNK:C	2.50	0.52
2:M5:62:UNK:CB	2:M5:64:UNK:N	2.73	0.52
2:M5:190:UNK:N	2:M5:191:UNK:C	2.73	0.52
1:L6:77:UNK:CA	1:L6:78:UNK:CB	2.84	0.52
2:M6:190:UNK:N	2:M6:191:UNK:C	2.73	0.52
1:L1:161:UNK:CB	1:L1:162:UNK:HA	2.40	0.52
1:L1:163:UNK:C	1:L1:165:UNK:N	2.69	0.52
2:M1:3:UNK:H	2:M1:6:UNK:CB	2.22	0.52
2:M1:113:UNK:CA	2:M1:114:UNK:C	2.85	0.52
11:u1:5:UNK:O	11:u1:8:UNK:N	2.42	0.52
13:w1:3:UNK:O	13:w1:4:UNK:C	2.56	0.52
2:M2:22:UNK:HA	2:M2:23:UNK:CB	2.40	0.52
2:M3:190:UNK:N	2:M3:191:UNK:C	2.73	0.52
12:v3:21:UNK:O	12:v3:25:UNK:N	2.42	0.52
1:L4:257:UNK:O	1:L4:261:UNK:N	2.43	0.52
2:M4:227:UNK:N	2:M4:228:UNK:CB	2.72	0.52
1:L5:60:UNK:O	1:L5:81:UNK:N	2.43	0.52
2:M5:3:UNK:H	2:M5:6:UNK:CB	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L6:82:UNK:N	1:L6:86:UNK:CB	2.73	0.52
1:L6:257:UNK:O	1:L6:261:UNK:N	2.43	0.52
1:L1:65:UNK:CB	1:L1:66:UNK:C	2.83	0.52
1:L1:161:UNK:HA	1:L1:163:UNK:CA	2.38	0.52
1:L1:257:UNK:O	1:L1:261:UNK:N	2.43	0.52
2:M1:309:UNK:O	2:M1:312:UNK:N	2.43	0.52
1:L2:60:UNK:O	1:L2:81:UNK:N	2.43	0.52
2:M2:3:UNK:H	2:M2:6:UNK:CB	2.22	0.52
2:M2:61:UNK:N	2:M2:62:UNK:C	2.73	0.52
1:L4:181:UNK:C	1:L4:183:UNK:N	2.71	0.52
2:M4:378:UNK:C	2:M4:380:UNK:N	2.72	0.52
7:U4:10:UNK:O	7:U4:13:UNK:N	2.43	0.52
10:t4:34:UNK:C	10:t4:36:UNK:N	2.68	0.52
1:L5:321:UNK:O	1:L5:324:UNK:C	2.58	0.52
2:M5:61:UNK:N	2:M5:62:UNK:C	2.73	0.52
8:n5:25:UNK:O	8:n5:28:UNK:N	2.42	0.52
12:v5:21:UNK:O	12:v5:25:UNK:N	2.42	0.52
1:L6:70:UNK:O	1:L6:73:UNK:O	2.28	0.52
2:M6:27:UNK:O	2:M6:28:UNK:C	2.58	0.52
2:M6:114:UNK:N	2:M6:177:UNK:CB	2.73	0.52
2:M6:328:UNK:O	2:M6:329:UNK:C	2.52	0.52
1:L1:241:UNK:O	1:L1:244:UNK:CB	2.57	0.51
1:L1:321:UNK:O	1:L1:324:UNK:C	2.58	0.51
2:M1:114:UNK:N	2:M1:177:UNK:CB	2.72	0.51
1:L2:279:UNK:O	1:L2:282:UNK:N	2.43	0.51
2:M2:63:UNK:O	2:M2:67:UNK:N	2.44	0.51
2:M2:190:UNK:N	2:M2:191:UNK:C	2.73	0.51
2:M2:309:UNK:O	2:M2:312:UNK:N	2.43	0.51
2:M3:309:UNK:O	2:M3:312:UNK:N	2.43	0.51
2:M4:139:UNK:HA	2:M4:140:UNK:CB	2.39	0.51
8:n4:25:UNK:O	8:n4:28:UNK:N	2.42	0.51
12:v4:21:UNK:O	12:v4:25:UNK:N	2.42	0.51
1:L5:70:UNK:O	1:L5:73:UNK:O	2.28	0.51
2:M5:22:UNK:HA	2:M5:23:UNK:CB	2.40	0.51
7:U5:10:UNK:O	7:U5:13:UNK:N	2.43	0.51
2:M6:115:UNK:N	2:M6:175:UNK:CB	2.73	0.51
7:U6:37:UNK:HA	7:U6:42:UNK:CB	2.39	0.51
1:L1:70:UNK:O	1:L1:73:UNK:O	2.28	0.51
2:M1:62:UNK:CB	2:M1:64:UNK:N	2.73	0.51
2:M1:347:UNK:HA	2:M1:415:UNK:HA	1.92	0.51
1:L2:257:UNK:O	1:L2:261:UNK:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:t2:33:UNK:O	10:t2:36:UNK:N	2.44	0.51
12:v2:3:UNK:O	12:v2:5:UNK:N	2.43	0.51
10:t3:33:UNK:O	10:t3:36:UNK:N	2.44	0.51
1:L4:82:UNK:N	1:L4:86:UNK:CB	2.73	0.51
2:M4:62:UNK:CB	2:M4:64:UNK:N	2.73	0.51
2:M4:190:UNK:N	2:M4:191:UNK:C	2.73	0.51
2:M5:115:UNK:N	2:M5:175:UNK:CB	2.73	0.51
12:v5:3:UNK:O	12:v5:5:UNK:N	2.43	0.51
1:L6:321:UNK:O	1:L6:324:UNK:C	2.58	0.51
12:v6:2:UNK:O	12:v6:5:UNK:CB	2.59	0.51
2:M1:115:UNK:N	2:M1:175:UNK:CB	2.73	0.51
2:M2:256:UNK:O	2:M2:257:UNK:C	2.56	0.51
1:L3:60:UNK:O	1:L3:81:UNK:N	2.43	0.51
2:M3:62:UNK:CB	2:M3:64:UNK:N	2.73	0.51
2:M3:63:UNK:O	2:M3:67:UNK:N	2.44	0.51
2:M3:341:UNK:C	2:M3:342:UNK:O	2.56	0.51
10:t3:34:UNK:C	10:t3:36:UNK:N	2.68	0.51
12:v3:14:UNK:O	12:v3:17:UNK:CB	2.59	0.51
1:L4:60:UNK:O	1:L4:81:UNK:N	2.43	0.51
2:M4:114:UNK:N	2:M4:177:UNK:CB	2.72	0.51
2:M4:393:UNK:O	2:M4:394:UNK:C	2.57	0.51
3:i4:22:UNK:C	3:i4:24:UNK:N	2.71	0.51
12:v4:2:UNK:O	12:v4:5:UNK:CB	2.59	0.51
2:M5:23:UNK:C	2:M5:25:UNK:N	2.74	0.51
2:M5:256:UNK:O	2:M5:257:UNK:C	2.56	0.51
12:v1:14:UNK:O	12:v1:17:UNK:CB	2.59	0.51
1:L2:207:UNK:CB	1:L2:209:UNK:CA	2.89	0.51
2:M2:139:UNK:HA	2:M2:140:UNK:CB	2.39	0.51
8:n2:53:UNK:O	8:n2:54:UNK:C	2.59	0.51
1:L3:70:UNK:O	1:L3:73:UNK:O	2.28	0.51
1:L3:257:UNK:O	1:L3:261:UNK:N	2.43	0.51
1:L3:321:UNK:O	1:L3:324:UNK:C	2.58	0.51
2:M3:27:UNK:O	2:M3:28:UNK:C	2.58	0.51
12:v3:2:UNK:O	12:v3:5:UNK:CB	2.59	0.51
12:v3:3:UNK:O	12:v3:5:UNK:N	2.43	0.51
1:L5:161:UNK:HA	1:L5:163:UNK:CA	2.38	0.51
2:M5:309:UNK:O	2:M5:312:UNK:N	2.43	0.51
12:v5:14:UNK:O	12:v5:17:UNK:CB	2.59	0.51
2:M6:139:UNK:HA	2:M6:140:UNK:CB	2.39	0.51
13:w6:26:UNK:O	13:w6:27:UNK:C	2.57	0.51
2:M1:27:UNK:O	2:M1:28:UNK:C	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M1:378:UNK:C	2:M1:380:UNK:N	2.72	0.51
1:L4:70:UNK:O	1:L4:73:UNK:O	2.28	0.51
2:M4:115:UNK:N	2:M4:175:UNK:CB	2.73	0.51
2:M4:347:UNK:HA	2:M4:415:UNK:HA	1.92	0.51
1:L6:161:UNK:HA	1:L6:163:UNK:CA	2.38	0.51
1:L6:163:UNK:C	1:L6:165:UNK:N	2.69	0.51
1:L1:60:UNK:O	1:L1:81:UNK:N	2.43	0.51
1:L2:55:UNK:N	1:L2:56:UNK:C	2.71	0.51
12:v2:14:UNK:O	12:v2:17:UNK:CB	2.59	0.51
2:M3:61:UNK:N	2:M3:62:UNK:C	2.73	0.51
2:M3:115:UNK:N	2:M3:175:UNK:CB	2.73	0.51
1:L5:323:UNK:CB	1:L5:475:UNK:CB	2.88	0.51
1:L6:207:UNK:CB	1:L6:209:UNK:CA	2.89	0.51
8:n6:53:UNK:O	8:n6:54:UNK:C	2.59	0.51
11:u6:5:UNK:O	11:u6:8:UNK:N	2.43	0.51
12:v2:2:UNK:O	12:v2:5:UNK:CB	2.59	0.51
1:L3:47:UNK:O	1:L3:48:UNK:C	2.53	0.51
1:L4:207:UNK:CB	1:L4:209:UNK:CA	2.89	0.51
1:L4:321:UNK:O	1:L4:324:UNK:C	2.58	0.51
2:M4:3:UNK:H	2:M4:6:UNK:CB	2.22	0.51
2:M4:348:UNK:N	2:M4:415:UNK:CB	2.74	0.51
2:M5:348:UNK:N	2:M5:415:UNK:CB	2.74	0.51
10:t5:33:UNK:O	10:t5:36:UNK:N	2.44	0.51
2:M6:347:UNK:HA	2:M6:415:UNK:HA	1.92	0.51
2:M1:341:UNK:C	2:M1:342:UNK:O	2.56	0.51
14:BA:1613:UNK:C	14:BA:1617:UNK:CB	2.89	0.51
2:M2:348:UNK:N	2:M2:415:UNK:CB	2.74	0.51
13:w2:3:UNK:O	13:w2:4:UNK:C	2.56	0.51
14:BB:1613:UNK:C	14:BB:1617:UNK:CB	2.89	0.51
2:M3:139:UNK:HA	2:M3:140:UNK:CB	2.39	0.51
2:M3:241:UNK:C	2:M3:243:UNK:N	2.71	0.51
2:M3:378:UNK:C	2:M3:380:UNK:N	2.72	0.51
2:M4:22:UNK:HA	2:M4:23:UNK:CB	2.40	0.51
3:i4:23:UNK:O	3:i4:26:UNK:N	2.44	0.51
1:L5:257:UNK:O	1:L5:261:UNK:N	2.43	0.51
2:M5:63:UNK:O	2:M5:67:UNK:N	2.44	0.51
8:n5:53:UNK:O	8:n5:54:UNK:C	2.59	0.51
12:v5:2:UNK:O	12:v5:5:UNK:CB	2.59	0.51
1:L6:60:UNK:O	1:L6:81:UNK:N	2.43	0.51
1:L6:190:UNK:HA	1:L6:194:UNK:CA	2.40	0.51
2:M6:348:UNK:N	2:M6:415:UNK:CB	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:v6:3:UNK:O	12:v6:5:UNK:N	2.43	0.51
12:v6:14:UNK:O	12:v6:17:UNK:CB	2.59	0.51
14:BF:1613:UNK:C	14:BF:1617:UNK:CB	2.89	0.51
2:M1:63:UNK:O	2:M1:67:UNK:N	2.43	0.51
2:M1:343:UNK:C	2:M1:345:UNK:N	2.71	0.51
10:t1:33:UNK:O	10:t1:36:UNK:N	2.44	0.51
2:M4:392:UNK:C	2:M4:394:UNK:N	2.68	0.51
8:n5:5:UNK:O	8:n5:8:UNK:CB	2.59	0.51
2:M6:22:UNK:HA	2:M6:23:UNK:CB	2.40	0.51
7:U1:10:UNK:O	7:U1:13:UNK:N	2.43	0.51
12:v1:2:UNK:O	12:v1:5:UNK:CB	2.59	0.51
1:L3:246:UNK:O	1:L3:250:UNK:N	2.44	0.51
2:M3:348:UNK:N	2:M3:415:UNK:CB	2.74	0.51
2:M3:384:UNK:C	2:M3:386:UNK:N	2.72	0.51
7:U3:10:UNK:O	7:U3:13:UNK:N	2.43	0.51
1:L4:47:UNK:C	1:L4:49:UNK:N	2.71	0.51
1:L4:288:UNK:CB	1:L4:308:UNK:CA	2.89	0.51
8:n4:5:UNK:O	8:n4:8:UNK:CB	2.59	0.51
10:t4:33:UNK:O	10:t4:36:UNK:N	2.44	0.51
1:L5:246:UNK:O	1:L5:250:UNK:N	2.44	0.51
3:i1:23:UNK:O	3:i1:26:UNK:N	2.44	0.50
1:L2:321:UNK:O	1:L2:324:UNK:C	2.58	0.50
2:M2:341:UNK:C	2:M2:342:UNK:O	2.56	0.50
1:L3:207:UNK:CB	1:L3:209:UNK:CA	2.89	0.50
2:M4:63:UNK:O	2:M4:67:UNK:N	2.44	0.50
2:M5:139:UNK:HA	2:M5:140:UNK:CB	2.39	0.50
2:M6:63:UNK:O	2:M6:67:UNK:N	2.44	0.50
1:L2:246:UNK:O	1:L2:250:UNK:N	2.44	0.50
8:n2:10:UNK:C	8:n2:12:UNK:N	2.67	0.50
1:L3:161:UNK:HA	1:L3:163:UNK:CA	2.38	0.50
2:M3:347:UNK:HA	2:M3:415:UNK:HA	1.92	0.50
2:M3:392:UNK:C	2:M3:394:UNK:N	2.68	0.50
2:M4:27:UNK:O	2:M4:28:UNK:C	2.58	0.50
8:n4:53:UNK:O	8:n4:54:UNK:C	2.59	0.50
12:v4:14:UNK:O	12:v4:17:UNK:CB	2.59	0.50
2:M5:391:UNK:O	2:M5:392:UNK:CB	2.56	0.50
2:M6:23:UNK:C	2:M6:25:UNK:N	2.74	0.50
2:M6:241:UNK:C	2:M6:243:UNK:N	2.71	0.50
2:M6:384:UNK:C	2:M6:386:UNK:N	2.72	0.50
10:t6:33:UNK:O	10:t6:36:UNK:N	2.44	0.50
2:M1:227:UNK:CB	2:M1:228:UNK:CB	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M2:378:UNK:C	2:M2:380:UNK:N	2.72	0.50
7:U2:10:UNK:O	7:U2:13:UNK:N	2.43	0.50
8:n2:5:UNK:O	8:n2:8:UNK:CB	2.59	0.50
1:L3:52:UNK:C	1:L3:54:UNK:N	2.73	0.50
1:L4:65:UNK:CB	1:L4:66:UNK:C	2.83	0.50
1:L5:161:UNK:CB	1:L5:162:UNK:CA	2.90	0.50
1:L6:181:UNK:C	1:L6:183:UNK:N	2.71	0.50
1:L1:94:UNK:O	1:L1:95:UNK:C	2.56	0.50
1:L1:161:UNK:CB	1:L1:162:UNK:CA	2.90	0.50
1:L1:207:UNK:CB	1:L1:209:UNK:CA	2.89	0.50
2:M3:328:UNK:O	2:M3:329:UNK:C	2.52	0.50
8:n3:5:UNK:O	8:n3:8:UNK:CB	2.59	0.50
14:BC:1613:UNK:C	14:BC:1617:UNK:CB	2.89	0.50
1:L4:105:UNK:O	1:L4:109:UNK:N	2.45	0.50
1:L4:161:UNK:CB	1:L4:162:UNK:CA	2.90	0.50
1:L4:246:UNK:O	1:L4:250:UNK:N	2.44	0.50
7:U6:22:UNK:CA	14:BF:1635:UNK:CB	2.88	0.50
2:M1:22:UNK:HA	2:M1:23:UNK:CB	2.40	0.50
2:M1:348:UNK:N	2:M1:415:UNK:CB	2.74	0.50
8:n1:5:UNK:O	8:n1:8:UNK:CB	2.59	0.50
8:n1:52:UNK:O	8:n1:55:UNK:CB	2.60	0.50
1:L2:70:UNK:O	1:L2:73:UNK:O	2.28	0.50
2:M2:227:UNK:CB	2:M2:228:UNK:CB	2.90	0.50
7:U2:22:UNK:CA	14:BB:1635:UNK:CB	2.88	0.50
1:L3:288:UNK:CB	1:L3:308:UNK:CA	2.89	0.50
2:M3:22:UNK:HA	2:M3:23:UNK:CB	2.40	0.50
2:M3:227:UNK:CB	2:M3:228:UNK:CB	2.90	0.50
2:M3:343:UNK:C	2:M3:345:UNK:N	2.71	0.50
8:n3:53:UNK:O	8:n3:54:UNK:C	2.59	0.50
2:M4:106:UNK:O	2:M4:109:UNK:N	2.45	0.50
1:L5:105:UNK:O	1:L5:109:UNK:N	2.45	0.50
3:i5:23:UNK:O	3:i5:26:UNK:N	2.44	0.50
8:n5:52:UNK:O	8:n5:55:UNK:CB	2.60	0.50
1:L6:47:UNK:C	1:L6:49:UNK:N	2.71	0.50
1:L6:105:UNK:O	1:L6:109:UNK:N	2.45	0.50
1:L6:306:UNK:O	1:L6:307:UNK:C	2.60	0.50
2:M6:227:UNK:CB	2:M6:228:UNK:CB	2.90	0.50
7:U6:10:UNK:O	7:U6:13:UNK:N	2.43	0.50
2:M1:23:UNK:C	2:M1:25:UNK:N	2.74	0.50
1:L2:263:UNK:O	1:L2:264:UNK:C	2.60	0.50
3:i2:22:UNK:C	3:i2:24:UNK:N	2.71	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:288:UNK:CB	1:L5:308:UNK:CA	2.89	0.50
2:M5:227:UNK:CB	2:M5:228:UNK:CB	2.90	0.50
2:M1:384:UNK:C	2:M1:386:UNK:N	2.72	0.50
2:M2:23:UNK:C	2:M2:25:UNK:N	2.74	0.50
2:M2:27:UNK:O	2:M2:28:UNK:C	2.58	0.50
3:i2:23:UNK:O	3:i2:26:UNK:N	2.44	0.50
1:L3:105:UNK:O	1:L3:109:UNK:N	2.45	0.50
10:t3:53:UNK:O	10:t3:54:UNK:C	2.58	0.50
13:w3:3:UNK:O	13:w3:4:UNK:C	2.56	0.50
14:BC:1609:UNK:O	14:BC:1613:UNK:N	2.45	0.50
2:M4:189:UNK:N	2:M4:191:UNK:C	2.75	0.50
4:g4:16:UNK:C	4:g4:18:UNK:N	2.67	0.50
1:L5:207:UNK:CB	1:L5:209:UNK:CA	2.89	0.50
1:L6:29:UNK:CA	1:L6:32:UNK:CB	2.86	0.50
1:L6:65:UNK:CB	1:L6:66:UNK:C	2.83	0.50
3:i6:23:UNK:O	3:i6:26:UNK:N	2.44	0.50
1:L1:288:UNK:CB	1:L1:308:UNK:CA	2.89	0.50
2:M1:396:UNK:O	2:M1:399:UNK:N	2.45	0.50
4:g1:15:UNK:O	4:g1:18:UNK:CB	2.60	0.50
3:i1:22:UNK:C	3:i1:24:UNK:N	2.71	0.50
2:M2:347:UNK:HA	2:M2:415:UNK:HA	1.92	0.50
1:L3:163:UNK:C	1:L3:165:UNK:N	2.69	0.50
2:M3:23:UNK:C	2:M3:25:UNK:N	2.74	0.50
2:M3:106:UNK:O	2:M3:109:UNK:N	2.45	0.50
1:L4:29:UNK:CA	1:L4:32:UNK:CB	2.86	0.50
8:n4:52:UNK:O	8:n4:55:UNK:CB	2.60	0.50
14:BD:1613:UNK:C	14:BD:1617:UNK:CB	2.89	0.50
14:BE:1613:UNK:C	14:BE:1617:UNK:CB	2.89	0.50
14:BF:1609:UNK:O	14:BF:1613:UNK:N	2.45	0.50
14:BA:1609:UNK:O	14:BA:1613:UNK:N	2.45	0.50
1:L3:29:UNK:CA	1:L3:32:UNK:CB	2.86	0.50
1:L4:263:UNK:O	1:L4:264:UNK:C	2.60	0.50
1:L4:306:UNK:O	1:L4:307:UNK:C	2.60	0.50
1:L5:47:UNK:C	1:L5:49:UNK:N	2.71	0.50
1:L6:241:UNK:O	1:L6:244:UNK:N	2.45	0.50
2:M6:106:UNK:O	2:M6:109:UNK:N	2.45	0.50
2:M6:287:UNK:O	2:M6:288:UNK:C	2.57	0.50
8:n6:5:UNK:O	8:n6:8:UNK:CB	2.59	0.50
2:M1:241:UNK:C	2:M1:243:UNK:N	2.71	0.49
12:v1:3:UNK:O	12:v1:5:UNK:N	2.43	0.49
8:n2:52:UNK:O	8:n2:55:UNK:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n3:44:UNK:O	8:n3:45:UNK:C	2.55	0.49
12:v3:14:UNK:O	12:v3:18:UNK:N	2.45	0.49
2:M4:23:UNK:C	2:M4:25:UNK:N	2.74	0.49
1:L5:306:UNK:O	1:L5:307:UNK:C	2.60	0.49
1:L6:52:UNK:C	1:L6:54:UNK:N	2.73	0.49
1:L1:190:UNK:HA	1:L1:194:UNK:CA	2.40	0.49
1:L2:105:UNK:O	1:L2:109:UNK:N	2.45	0.49
4:g2:15:UNK:O	4:g2:18:UNK:CB	2.60	0.49
2:M3:396:UNK:O	2:M3:399:UNK:N	2.45	0.49
3:i3:23:UNK:O	3:i3:26:UNK:N	2.44	0.49
5:s4:11:UNK:O	5:s4:14:UNK:CB	2.60	0.49
12:v4:3:UNK:O	12:v4:5:UNK:N	2.43	0.49
2:M5:189:UNK:N	2:M5:191:UNK:C	2.75	0.49
1:L6:48:UNK:O	1:L6:52:UNK:N	2.46	0.49
1:L6:246:UNK:O	1:L6:250:UNK:N	2.44	0.49
4:g6:15:UNK:O	4:g6:18:UNK:CB	2.60	0.49
2:M1:106:UNK:O	2:M1:109:UNK:N	2.45	0.49
14:BB:1609:UNK:O	14:BB:1613:UNK:N	2.45	0.49
2:M5:106:UNK:O	2:M5:109:UNK:N	2.45	0.49
5:s5:11:UNK:O	5:s5:14:UNK:CB	2.60	0.49
13:w5:26:UNK:O	13:w5:27:UNK:C	2.57	0.49
1:L6:288:UNK:CB	1:L6:308:UNK:CA	2.89	0.49
2:M6:180:UNK:C	2:M6:182:UNK:N	2.65	0.49
2:M6:396:UNK:O	2:M6:399:UNK:N	2.45	0.49
1:L1:137:UNK:O	1:L1:140:UNK:CB	2.61	0.49
1:L1:263:UNK:O	1:L1:264:UNK:C	2.60	0.49
5:s1:11:UNK:O	5:s1:14:UNK:CB	2.60	0.49
1:L2:241:UNK:O	1:L2:244:UNK:N	2.45	0.49
1:L4:241:UNK:O	1:L4:244:UNK:N	2.45	0.49
14:BD:1609:UNK:O	14:BD:1613:UNK:N	2.45	0.49
1:L5:263:UNK:O	1:L5:264:UNK:C	2.60	0.49
4:g5:16:UNK:C	4:g5:18:UNK:N	2.67	0.49
1:L6:137:UNK:O	1:L6:140:UNK:CB	2.60	0.49
1:L6:161:UNK:CB	1:L6:162:UNK:CA	2.90	0.49
2:M6:378:UNK:C	2:M6:380:UNK:N	2.72	0.49
1:L1:241:UNK:O	1:L1:244:UNK:N	2.45	0.49
1:L1:297:UNK:CA	1:L1:356:UNK:N	2.73	0.49
1:L3:48:UNK:O	1:L3:52:UNK:N	2.46	0.49
1:L3:137:UNK:O	1:L3:140:UNK:CB	2.61	0.49
2:M3:348:UNK:CA	2:M3:351:UNK:CB	2.85	0.49
1:L5:241:UNK:O	1:L5:244:UNK:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:v5:14:UNK:O	12:v5:18:UNK:N	2.45	0.49
1:L1:246:UNK:O	1:L1:250:UNK:N	2.44	0.49
1:L2:161:UNK:HA	1:L2:163:UNK:CA	2.38	0.49
1:L2:288:UNK:CB	1:L2:308:UNK:CA	2.89	0.49
2:M2:106:UNK:O	2:M2:109:UNK:N	2.45	0.49
5:s2:11:UNK:O	5:s2:14:UNK:CB	2.60	0.49
1:L3:190:UNK:HA	1:L3:194:UNK:CA	2.40	0.49
1:L4:137:UNK:O	1:L4:140:UNK:CB	2.60	0.49
2:M4:227:UNK:CB	2:M4:228:UNK:CB	2.90	0.49
2:M4:396:UNK:O	2:M4:399:UNK:N	2.45	0.49
12:v4:14:UNK:O	12:v4:18:UNK:N	2.45	0.49
1:L5:137:UNK:O	1:L5:140:UNK:CB	2.60	0.49
2:M5:392:UNK:C	2:M5:394:UNK:N	2.68	0.49
4:g5:15:UNK:O	4:g5:18:UNK:CB	2.60	0.49
1:L6:263:UNK:O	1:L6:264:UNK:C	2.60	0.49
8:n6:52:UNK:O	8:n6:55:UNK:CB	2.60	0.49
1:L1:48:UNK:O	1:L1:52:UNK:N	2.46	0.49
1:L2:48:UNK:O	1:L2:52:UNK:N	2.46	0.49
1:L2:161:UNK:CB	1:L2:162:UNK:CA	2.90	0.49
2:M2:287:UNK:O	2:M2:288:UNK:C	2.57	0.49
8:n3:52:UNK:O	8:n3:55:UNK:CB	2.60	0.49
1:L4:190:UNK:HA	1:L4:194:UNK:CA	2.40	0.49
7:U4:22:UNK:CA	14:BD:1635:UNK:CB	2.88	0.49
2:M5:396:UNK:O	2:M5:399:UNK:N	2.45	0.49
3:i5:22:UNK:C	3:i5:24:UNK:N	2.71	0.49
1:L6:281:UNK:CB	1:L6:315:UNK:CA	2.91	0.49
1:L1:105:UNK:O	1:L1:109:UNK:N	2.45	0.49
1:L3:94:UNK:O	1:L3:95:UNK:C	2.56	0.49
1:L3:161:UNK:CB	1:L3:162:UNK:CA	2.90	0.49
1:L3:241:UNK:O	1:L3:244:UNK:N	2.45	0.49
1:L4:48:UNK:O	1:L4:52:UNK:N	2.45	0.49
2:M4:275:UNK:C	2:M4:278:UNK:CB	2.91	0.49
4:g4:15:UNK:O	4:g4:18:UNK:CB	2.60	0.49
1:L1:29:UNK:CA	1:L1:32:UNK:CB	2.86	0.49
12:v1:14:UNK:O	12:v1:18:UNK:N	2.45	0.49
1:L3:281:UNK:CB	1:L3:315:UNK:CA	2.91	0.49
1:L3:477:UNK:C	1:L3:479:UNK:H	2.26	0.49
1:L5:52:UNK:C	1:L5:54:UNK:N	2.73	0.49
2:M5:341:UNK:C	2:M5:342:UNK:O	2.56	0.49
1:L6:477:UNK:C	1:L6:479:UNK:H	2.26	0.49
1:L2:65:UNK:CB	1:L2:66:UNK:C	2.83	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:281:UNK:CB	1:L2:315:UNK:CA	2.91	0.49
12:v2:14:UNK:O	12:v2:18:UNK:N	2.45	0.49
5:s6:21:UNK:O	5:s6:22:UNK:C	2.61	0.49
1:L1:181:UNK:C	1:L1:183:UNK:N	2.71	0.48
2:M1:275:UNK:C	2:M1:278:UNK:CB	2.91	0.48
4:g3:15:UNK:O	4:g3:18:UNK:CB	2.60	0.48
2:M4:14:UNK:O	2:M4:15:UNK:C	2.60	0.48
2:M6:275:UNK:C	2:M6:278:UNK:CB	2.91	0.48
5:s3:11:UNK:O	5:s3:14:UNK:CB	2.60	0.48
1:L4:477:UNK:C	1:L4:479:UNK:H	2.26	0.48
2:M4:63:UNK:O	2:M4:66:UNK:N	2.47	0.48
14:BE:1609:UNK:O	14:BE:1613:UNK:N	2.45	0.48
2:M6:63:UNK:O	2:M6:66:UNK:N	2.47	0.48
2:M1:448:UNK:O	2:M1:449:UNK:C	2.61	0.48
1:L2:137:UNK:O	1:L2:140:UNK:CB	2.60	0.48
2:M2:396:UNK:O	2:M2:399:UNK:N	2.45	0.48
1:L3:128:UNK:O	1:L3:129:UNK:C	2.61	0.48
2:M3:63:UNK:O	2:M3:66:UNK:N	2.47	0.48
2:M3:275:UNK:C	2:M3:278:UNK:CB	2.91	0.48
5:s4:21:UNK:O	5:s4:22:UNK:C	2.61	0.48
1:L5:48:UNK:O	1:L5:52:UNK:N	2.46	0.48
1:L1:281:UNK:CB	1:L1:315:UNK:CA	2.91	0.48
13:w1:16:UNK:O	13:w1:20:UNK:N	2.47	0.48
1:L2:163:UNK:C	1:L2:165:UNK:N	2.69	0.48
2:M2:275:UNK:C	2:M2:278:UNK:CB	2.91	0.48
1:L3:263:UNK:O	1:L3:264:UNK:C	2.60	0.48
1:L4:281:UNK:CB	1:L4:315:UNK:CA	2.91	0.48
2:M4:341:UNK:C	2:M4:342:UNK:O	2.56	0.48
2:M5:63:UNK:O	2:M5:66:UNK:N	2.47	0.48
2:M5:386:UNK:HA	2:M5:390:UNK:HA	1.96	0.48
5:s6:11:UNK:O	5:s6:14:UNK:CB	2.60	0.48
12:v6:14:UNK:O	12:v6:18:UNK:N	2.45	0.48
1:L2:306:UNK:O	1:L2:307:UNK:C	2.60	0.48
3:h2:12:UNK:O	3:h2:15:UNK:CB	2.62	0.48
2:M3:127:UNK:O	2:M3:128:UNK:C	2.61	0.48
2:M3:448:UNK:O	2:M3:449:UNK:C	2.61	0.48
2:M4:133:UNK:C	2:M4:224:UNK:CB	2.92	0.48
13:w4:16:UNK:O	13:w4:20:UNK:N	2.47	0.48
1:L5:281:UNK:CB	1:L5:315:UNK:CA	2.91	0.48
2:M6:14:UNK:O	2:M6:15:UNK:C	2.60	0.48
10:t1:53:UNK:O	10:t1:54:UNK:C	2.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M2:63:UNK:O	2:M2:66:UNK:N	2.47	0.48
3:h4:12:UNK:O	3:h4:15:UNK:CB	2.62	0.48
14:BD:547:UNK:O	14:BE:1589:UNK:C	2.56	0.48
1:L5:477:UNK:C	1:L5:479:UNK:H	2.26	0.48
1:L6:297:UNK:CA	1:L6:356:UNK:N	2.73	0.48
2:M6:133:UNK:C	2:M6:224:UNK:CB	2.92	0.48
8:n6:44:UNK:O	8:n6:45:UNK:C	2.55	0.48
13:w6:16:UNK:O	13:w6:20:UNK:N	2.47	0.48
2:M1:127:UNK:O	2:M1:128:UNK:C	2.61	0.48
2:M1:189:UNK:N	2:M1:191:UNK:C	2.75	0.48
8:n1:44:UNK:O	8:n1:45:UNK:C	2.55	0.48
13:w2:16:UNK:O	13:w2:20:UNK:N	2.47	0.48
2:M3:386:UNK:HA	2:M3:390:UNK:HA	1.96	0.48
3:h3:12:UNK:O	3:h3:15:UNK:CB	2.62	0.48
5:s3:21:UNK:O	5:s3:22:UNK:C	2.61	0.48
1:L4:163:UNK:C	1:L4:165:UNK:N	2.69	0.48
2:M6:133:UNK:HA	2:M6:224:UNK:CB	2.44	0.48
1:L1:47:UNK:C	1:L1:49:UNK:N	2.71	0.48
2:M4:348:UNK:CA	2:M4:351:UNK:CB	2.85	0.48
2:M4:386:UNK:HA	2:M4:390:UNK:HA	1.96	0.48
1:L5:181:UNK:C	1:L5:183:UNK:N	2.71	0.48
2:M5:133:UNK:C	2:M5:224:UNK:CB	2.92	0.48
2:M5:275:UNK:C	2:M5:278:UNK:CB	2.91	0.48
8:n1:53:UNK:O	8:n1:54:UNK:C	2.59	0.48
1:L2:339:UNK:O	1:L2:342:UNK:N	2.47	0.48
2:M2:347:UNK:C	2:M2:351:UNK:CB	2.92	0.48
2:M2:448:UNK:O	2:M2:449:UNK:C	2.61	0.48
13:w3:16:UNK:O	13:w3:20:UNK:N	2.47	0.48
2:M4:133:UNK:CB	2:M4:224:UNK:CB	2.92	0.48
1:L6:339:UNK:O	1:L6:342:UNK:N	2.47	0.48
2:M1:133:UNK:C	2:M1:224:UNK:CB	2.92	0.48
2:M2:14:UNK:O	2:M2:15:UNK:C	2.60	0.48
2:M2:133:UNK:CB	2:M2:224:UNK:CB	2.92	0.48
2:M2:348:UNK:CA	2:M2:351:UNK:CB	2.85	0.48
2:M2:384:UNK:C	2:M2:386:UNK:N	2.72	0.48
1:L3:47:UNK:C	1:L3:49:UNK:N	2.71	0.48
3:f3:18:UNK:O	3:f3:22:UNK:N	2.47	0.48
2:M1:133:UNK:CB	2:M1:224:UNK:CB	2.92	0.47
2:M1:133:UNK:HA	2:M1:224:UNK:CB	2.44	0.47
2:M1:386:UNK:HA	2:M1:390:UNK:HA	1.96	0.47
7:U1:22:UNK:CA	14:BA:1635:UNK:CB	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:239:UNK:C	1:L2:240:UNK:O	2.60	0.47
1:L2:477:UNK:C	1:L2:479:UNK:H	2.26	0.47
3:f2:18:UNK:O	3:f2:22:UNK:N	2.47	0.47
14:BB:1609:UNK:O	14:BB:1613:UNK:CB	2.62	0.47
2:M3:14:UNK:O	2:M3:15:UNK:C	2.60	0.47
2:M3:133:UNK:CB	2:M3:224:UNK:CB	2.92	0.47
1:L4:128:UNK:O	1:L4:129:UNK:C	2.61	0.47
2:M1:14:UNK:O	2:M1:15:UNK:C	2.60	0.47
10:t1:9:UNK:O	10:t1:10:UNK:C	2.61	0.47
1:L2:450:UNK:O	1:L2:453:UNK:N	2.47	0.47
5:s2:21:UNK:O	5:s2:22:UNK:C	2.61	0.47
1:L3:339:UNK:O	1:L3:342:UNK:N	2.47	0.47
2:M3:133:UNK:C	2:M3:224:UNK:CB	2.92	0.47
2:M4:127:UNK:O	2:M4:128:UNK:C	2.61	0.47
2:M4:384:UNK:C	2:M4:386:UNK:N	2.72	0.47
2:M6:448:UNK:O	2:M6:449:UNK:C	2.61	0.47
3:f6:18:UNK:O	3:f6:22:UNK:N	2.47	0.47
1:L1:128:UNK:O	1:L1:129:UNK:C	2.61	0.47
1:L1:306:UNK:O	1:L1:307:UNK:C	2.60	0.47
1:L1:339:UNK:O	1:L1:342:UNK:N	2.47	0.47
2:M1:63:UNK:O	2:M1:66:UNK:N	2.47	0.47
2:M1:351:UNK:O	2:M1:352:UNK:CB	2.62	0.47
14:BA:1609:UNK:O	14:BA:1613:UNK:CB	2.62	0.47
2:M2:127:UNK:O	2:M2:128:UNK:C	2.61	0.47
14:BB:1625:UNK:O	14:BB:1626:UNK:O	2.33	0.47
2:M5:351:UNK:O	2:M5:352:UNK:CB	2.62	0.47
13:w5:16:UNK:O	13:w5:20:UNK:N	2.47	0.47
1:L6:111:UNK:O	1:L6:114:UNK:N	2.47	0.47
2:M1:392:UNK:C	2:M1:394:UNK:N	2.68	0.47
3:h1:12:UNK:O	3:h1:15:UNK:CB	2.62	0.47
2:M2:133:UNK:HA	2:M2:224:UNK:CB	2.44	0.47
2:M2:351:UNK:O	2:M2:352:UNK:CB	2.62	0.47
2:M3:133:UNK:HA	2:M3:224:UNK:CB	2.44	0.47
10:t4:53:UNK:O	10:t4:54:UNK:C	2.58	0.47
2:M6:188:UNK:CB	2:M6:189:UNK:CA	2.93	0.47
3:h6:12:UNK:O	3:h6:15:UNK:CB	2.62	0.47
2:M2:386:UNK:HA	2:M2:390:UNK:HA	1.96	0.47
8:n2:10:UNK:O	8:n2:13:UNK:CB	2.63	0.47
10:t2:9:UNK:O	10:t2:10:UNK:C	2.61	0.47
1:L3:396:UNK:O	1:L3:399:UNK:N	2.48	0.47
4:g3:11:UNK:O	4:g3:13:UNK:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:52:UNK:C	1:L4:54:UNK:N	2.73	0.47
5:p4:11:UNK:C	5:p4:13:UNK:N	2.76	0.47
14:BD:1609:UNK:O	14:BD:1613:UNK:CB	2.62	0.47
1:L5:396:UNK:O	1:L5:399:UNK:N	2.48	0.47
2:M5:133:UNK:CB	2:M5:224:UNK:CB	2.92	0.47
3:h5:12:UNK:O	3:h5:15:UNK:CB	2.62	0.47
1:L6:396:UNK:O	1:L6:399:UNK:N	2.48	0.47
2:M6:140:UNK:C	2:M6:142:UNK:N	2.74	0.47
1:L1:207:UNK:HA	1:L1:208:UNK:C	2.45	0.47
3:f1:18:UNK:O	3:f1:22:UNK:N	2.47	0.47
1:L3:239:UNK:C	1:L3:240:UNK:O	2.60	0.47
1:L3:450:UNK:O	1:L3:453:UNK:N	2.47	0.47
2:M3:188:UNK:CB	2:M3:189:UNK:CA	2.93	0.47
2:M3:351:UNK:O	2:M3:352:UNK:CB	2.62	0.47
14:BC:1590:UNK:N	14:BF:547:UNK:CB	2.78	0.47
1:L4:339:UNK:O	1:L4:342:UNK:N	2.47	0.47
2:M4:106:UNK:HA	2:M4:109:UNK:CB	2.45	0.47
4:g4:11:UNK:O	4:g4:13:UNK:N	2.48	0.47
1:L5:190:UNK:HA	1:L5:194:UNK:CA	2.40	0.47
2:M5:347:UNK:C	2:M5:351:UNK:CB	2.92	0.47
14:BE:1625:UNK:O	14:BE:1626:UNK:O	2.33	0.47
1:L1:52:UNK:C	1:L1:54:UNK:N	2.73	0.47
1:L1:477:UNK:C	1:L1:479:UNK:H	2.26	0.47
5:p1:11:UNK:C	5:p1:13:UNK:N	2.76	0.47
14:BA:1625:UNK:O	14:BA:1626:UNK:O	2.33	0.47
1:L2:61:UNK:CA	1:L2:80:UNK:CB	2.93	0.47
1:L2:111:UNK:O	1:L2:114:UNK:N	2.48	0.47
1:L2:316:UNK:O	1:L2:317:UNK:C	2.63	0.47
1:L2:396:UNK:O	1:L2:399:UNK:N	2.48	0.47
2:M2:133:UNK:C	2:M2:224:UNK:CB	2.92	0.47
1:L5:339:UNK:O	1:L5:342:UNK:N	2.47	0.47
1:L5:450:UNK:O	1:L5:453:UNK:N	2.47	0.47
4:g5:11:UNK:O	4:g5:13:UNK:N	2.48	0.47
1:L6:61:UNK:CA	1:L6:80:UNK:CB	2.93	0.47
1:L6:450:UNK:O	1:L6:453:UNK:N	2.47	0.47
1:L1:111:UNK:O	1:L1:114:UNK:N	2.48	0.47
1:L1:450:UNK:O	1:L1:453:UNK:N	2.47	0.47
14:BB:1614:UNK:C	14:BB:1617:UNK:CA	2.88	0.47
2:M4:133:UNK:HA	2:M4:224:UNK:CB	2.44	0.47
2:M4:188:UNK:CB	2:M4:189:UNK:CA	2.93	0.47
2:M4:255:UNK:O	2:M4:258:UNK:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f4:18:UNK:O	3:f4:22:UNK:N	2.47	0.47
3:f5:18:UNK:O	3:f5:22:UNK:N	2.47	0.47
14:BE:1609:UNK:O	14:BE:1613:UNK:CB	2.62	0.47
2:M6:133:UNK:CB	2:M6:224:UNK:CB	2.92	0.47
14:BF:1609:UNK:O	14:BF:1613:UNK:CB	2.62	0.47
1:L1:452:UNK:O	1:L1:456:UNK:N	2.48	0.47
1:L2:95:UNK:O	1:L2:98:UNK:N	2.48	0.47
1:L2:297:UNK:CA	1:L2:356:UNK:N	2.73	0.47
2:M2:106:UNK:HA	2:M2:109:UNK:CB	2.45	0.47
2:M2:392:UNK:C	2:M2:394:UNK:N	2.68	0.47
1:L3:111:UNK:O	1:L3:114:UNK:N	2.48	0.47
8:n3:10:UNK:O	8:n3:13:UNK:CB	2.63	0.47
2:M4:347:UNK:C	2:M4:351:UNK:CB	2.92	0.47
2:M4:351:UNK:O	2:M4:352:UNK:CB	2.62	0.47
8:n4:10:UNK:O	8:n4:13:UNK:CB	2.63	0.47
14:BD:1625:UNK:O	14:BD:1626:UNK:O	2.33	0.47
1:L5:452:UNK:O	1:L5:456:UNK:N	2.48	0.47
2:M5:273:UNK:O	2:M5:277:UNK:N	2.48	0.47
8:n1:10:UNK:O	8:n1:13:UNK:CB	2.63	0.47
5:s1:21:UNK:O	5:s1:22:UNK:C	2.61	0.47
1:L2:190:UNK:HA	1:L2:194:UNK:CA	2.40	0.47
1:L2:207:UNK:HA	1:L2:208:UNK:C	2.45	0.47
2:M2:433:UNK:O	2:M2:434:UNK:C	2.62	0.47
2:M3:140:UNK:C	2:M3:142:UNK:N	2.74	0.47
2:M3:255:UNK:O	2:M3:258:UNK:CB	2.63	0.47
1:L5:95:UNK:O	1:L5:98:UNK:N	2.48	0.47
1:L5:111:UNK:O	1:L5:114:UNK:N	2.48	0.47
1:L5:207:UNK:HA	1:L5:208:UNK:C	2.45	0.47
1:L6:452:UNK:O	1:L6:456:UNK:N	2.48	0.47
2:M6:127:UNK:O	2:M6:128:UNK:C	2.61	0.47
8:n6:10:UNK:O	8:n6:13:UNK:CB	2.63	0.47
2:M1:188:UNK:CB	2:M1:189:UNK:CA	2.93	0.46
4:g1:11:UNK:O	4:g1:13:UNK:N	2.48	0.46
10:t2:53:UNK:O	10:t2:54:UNK:C	2.58	0.46
2:M3:168:UNK:CB	2:M3:174:UNK:CB	2.93	0.46
2:M3:189:UNK:N	2:M3:191:UNK:C	2.75	0.46
2:M3:273:UNK:O	2:M3:277:UNK:N	2.48	0.46
14:BC:1609:UNK:O	14:BC:1613:UNK:CB	2.62	0.46
1:L4:111:UNK:O	1:L4:114:UNK:N	2.48	0.46
1:L5:316:UNK:O	1:L5:317:UNK:C	2.63	0.46
2:M5:168:UNK:CB	2:M5:174:UNK:CB	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M5:255:UNK:O	2:M5:258:UNK:CB	2.63	0.46
8:n5:10:UNK:O	8:n5:13:UNK:CB	2.63	0.46
2:M6:106:UNK:HA	2:M6:109:UNK:CB	2.45	0.46
2:M6:157:UNK:O	2:M6:160:UNK:N	2.48	0.46
2:M6:255:UNK:O	2:M6:258:UNK:CB	2.63	0.46
2:M6:273:UNK:O	2:M6:276:UNK:N	2.49	0.46
10:t6:53:UNK:O	10:t6:54:UNK:C	2.58	0.46
1:L1:396:UNK:O	1:L1:399:UNK:N	2.48	0.46
2:M1:106:UNK:HA	2:M1:109:UNK:CB	2.45	0.46
2:M2:113:UNK:CA	2:M2:114:UNK:CB	2.89	0.46
2:M2:188:UNK:CB	2:M2:189:UNK:CA	2.93	0.46
4:g2:11:UNK:O	4:g2:13:UNK:N	2.48	0.46
1:L4:95:UNK:O	1:L4:98:UNK:N	2.48	0.46
5:j5:22:UNK:O	5:j5:25:UNK:N	2.48	0.46
1:L6:94:UNK:O	1:L6:95:UNK:C	2.56	0.46
4:g6:11:UNK:O	4:g6:13:UNK:N	2.48	0.46
5:j6:22:UNK:O	5:j6:25:UNK:N	2.48	0.46
12:v6:19:UNK:O	12:v6:23:UNK:N	2.49	0.46
1:L1:316:UNK:O	1:L1:317:UNK:C	2.63	0.46
14:BA:1614:UNK:C	14:BA:1617:UNK:CA	2.88	0.46
2:M2:140:UNK:C	2:M2:142:UNK:N	2.74	0.46
2:M3:106:UNK:HA	2:M3:109:UNK:CB	2.45	0.46
2:M3:281:UNK:O	2:M3:284:UNK:C	2.64	0.46
1:L4:297:UNK:CA	1:L4:356:UNK:N	2.73	0.46
1:L4:450:UNK:O	1:L4:453:UNK:N	2.47	0.46
2:M4:168:UNK:CB	2:M4:174:UNK:CB	2.93	0.46
2:M4:273:UNK:O	2:M4:277:UNK:N	2.48	0.46
2:M5:188:UNK:CB	2:M5:189:UNK:CA	2.93	0.46
3:i5:27:UNK:C	3:i5:28:UNK:O	2.56	0.46
7:U5:22:UNK:CA	14:BE:1635:UNK:CB	2.88	0.46
1:L6:95:UNK:O	1:L6:98:UNK:N	2.48	0.46
1:L6:128:UNK:O	1:L6:129:UNK:C	2.61	0.46
1:L6:225:UNK:C	1:L6:229:UNK:CB	2.93	0.46
14:BF:1625:UNK:O	14:BF:1626:UNK:O	2.33	0.46
1:L1:108:UNK:O	1:L1:111:UNK:N	2.49	0.46
2:M1:255:UNK:O	2:M1:258:UNK:CB	2.63	0.46
2:M1:281:UNK:O	2:M1:284:UNK:C	2.64	0.46
3:i1:27:UNK:C	3:i1:28:UNK:O	2.56	0.46
12:v1:10:UNK:O	12:v1:13:UNK:N	2.49	0.46
1:L2:52:UNK:C	1:L2:54:UNK:N	2.73	0.46
1:L2:271:UNK:O	1:L2:274:UNK:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:314:UNK:O	1:L2:317:UNK:N	2.49	0.46
2:M2:157:UNK:O	2:M2:160:UNK:N	2.48	0.46
2:M2:273:UNK:O	2:M2:276:UNK:N	2.49	0.46
1:L3:77:UNK:CA	1:L3:78:UNK:CB	2.84	0.46
1:L3:95:UNK:O	1:L3:98:UNK:N	2.48	0.46
2:M3:273:UNK:O	2:M3:276:UNK:N	2.49	0.46
1:L4:396:UNK:O	1:L4:399:UNK:N	2.48	0.46
2:M4:273:UNK:O	2:M4:276:UNK:N	2.49	0.46
1:L5:239:UNK:C	1:L5:240:UNK:O	2.60	0.46
10:t5:53:UNK:O	10:t5:54:UNK:C	2.58	0.46
1:L6:314:UNK:O	1:L6:317:UNK:N	2.49	0.46
1:L1:271:UNK:O	1:L1:274:UNK:N	2.49	0.46
1:L1:316:UNK:O	1:L1:319:UNK:CA	2.64	0.46
2:M2:273:UNK:O	2:M2:277:UNK:N	2.48	0.46
5:s2:23:UNK:O	5:s2:26:UNK:N	2.49	0.46
1:L3:314:UNK:O	1:L3:317:UNK:N	2.49	0.46
1:L3:316:UNK:O	1:L3:319:UNK:CA	2.64	0.46
2:M3:62:UNK:N	2:M3:63:UNK:CA	2.77	0.46
2:M4:157:UNK:O	2:M4:160:UNK:N	2.48	0.46
5:s4:23:UNK:O	5:s4:26:UNK:N	2.49	0.46
2:M5:106:UNK:HA	2:M5:109:UNK:CB	2.45	0.46
2:M5:384:UNK:C	2:M5:386:UNK:N	2.72	0.46
2:M6:351:UNK:O	2:M6:352:UNK:CB	2.62	0.46
12:v6:10:UNK:O	12:v6:13:UNK:N	2.49	0.46
2:M1:157:UNK:O	2:M1:160:UNK:N	2.48	0.46
1:L2:47:UNK:C	1:L2:49:UNK:N	2.71	0.46
2:M2:281:UNK:O	2:M2:284:UNK:C	2.64	0.46
1:L3:108:UNK:O	1:L3:111:UNK:N	2.49	0.46
1:L3:225:UNK:C	1:L3:229:UNK:CB	2.93	0.46
5:s3:23:UNK:O	5:s3:26:UNK:N	2.49	0.46
3:h4:10:UNK:C	3:h4:12:UNK:N	2.77	0.46
7:U4:55:UNK:O	7:U4:58:UNK:O	2.34	0.46
12:v4:10:UNK:O	12:v4:13:UNK:N	2.49	0.46
1:L5:61:UNK:CA	1:L5:80:UNK:CB	2.93	0.46
2:M5:157:UNK:O	2:M5:160:UNK:N	2.48	0.46
1:L6:108:UNK:O	1:L6:111:UNK:N	2.49	0.46
2:M1:87:UNK:HA	2:M1:89:UNK:HA	1.98	0.46
1:L2:225:UNK:C	1:L2:229:UNK:CB	2.93	0.46
2:M2:42:UNK:C	2:M2:44:UNK:N	2.76	0.46
5:p2:8:UNK:O	5:p2:9:UNK:C	2.64	0.46
12:v2:10:UNK:O	12:v2:13:UNK:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L3:306:UNK:O	1:L3:307:UNK:C	2.60	0.46
2:M3:38:UNK:O	2:M3:41:UNK:N	2.49	0.46
12:v3:10:UNK:O	12:v3:13:UNK:N	2.49	0.46
1:L4:225:UNK:C	1:L4:229:UNK:CB	2.93	0.46
2:M5:133:UNK:HA	2:M5:224:UNK:CB	2.44	0.46
2:M5:448:UNK:O	2:M5:449:UNK:C	2.61	0.46
3:f5:20:UNK:O	3:f5:24:UNK:CB	2.64	0.46
10:t5:9:UNK:O	10:t5:10:UNK:C	2.61	0.46
2:M6:281:UNK:O	2:M6:284:UNK:C	2.64	0.46
2:M6:386:UNK:HA	2:M6:390:UNK:HA	1.96	0.46
3:f6:20:UNK:O	3:f6:24:UNK:CB	2.64	0.46
10:t6:9:UNK:O	10:t6:10:UNK:C	2.62	0.46
1:L1:225:UNK:C	1:L1:229:UNK:CB	2.93	0.46
1:L2:316:UNK:O	1:L2:319:UNK:CA	2.64	0.46
2:M2:52:UNK:HA	2:M2:53:UNK:HA	1.71	0.46
2:M2:255:UNK:O	2:M2:258:UNK:CB	2.63	0.46
2:M2:327:UNK:O	2:M2:330:UNK:N	2.49	0.46
5:j2:22:UNK:O	5:j2:25:UNK:N	2.48	0.46
5:j3:22:UNK:O	5:j3:25:UNK:N	2.48	0.46
1:L4:207:UNK:HA	1:L4:208:UNK:C	2.45	0.46
1:L4:271:UNK:O	1:L4:274:UNK:N	2.49	0.46
1:L4:314:UNK:O	1:L4:317:UNK:N	2.49	0.46
5:j4:22:UNK:O	5:j4:25:UNK:N	2.48	0.46
1:L5:169:UNK:O	1:L5:173:UNK:N	2.49	0.46
1:L5:271:UNK:O	1:L5:274:UNK:N	2.49	0.46
2:M5:273:UNK:O	2:M5:276:UNK:N	2.48	0.46
2:M5:327:UNK:O	2:M5:330:UNK:N	2.49	0.46
12:v5:19:UNK:O	12:v5:23:UNK:N	2.49	0.46
2:M6:38:UNK:O	2:M6:41:UNK:N	2.49	0.46
2:M1:168:UNK:CB	2:M1:174:UNK:CB	2.93	0.46
5:j1:22:UNK:O	5:j1:25:UNK:N	2.49	0.46
12:v1:19:UNK:O	12:v1:23:UNK:N	2.49	0.46
1:L2:169:UNK:O	1:L2:173:UNK:N	2.49	0.46
2:M2:432:UNK:O	2:M2:435:UNK:N	2.49	0.46
12:v2:19:UNK:O	12:v2:23:UNK:N	2.49	0.46
1:L3:316:UNK:O	1:L3:317:UNK:C	2.63	0.46
2:M3:178:UNK:O	2:M3:179:UNK:C	2.63	0.46
2:M3:327:UNK:O	2:M3:330:UNK:N	2.49	0.46
3:f3:20:UNK:O	3:f3:24:UNK:CB	2.64	0.46
3:i3:27:UNK:C	3:i3:28:UNK:O	2.56	0.46
14:BC:1625:UNK:O	14:BC:1626:UNK:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:452:UNK:O	1:L4:456:UNK:N	2.48	0.46
2:M4:315:UNK:O	2:M4:316:UNK:C	2.64	0.46
1:L5:225:UNK:C	1:L5:229:UNK:CB	2.93	0.46
2:M5:38:UNK:O	2:M5:41:UNK:N	2.49	0.46
4:g5:9:UNK:O	4:g5:12:UNK:CB	2.64	0.46
1:L1:95:UNK:O	1:L1:98:UNK:N	2.48	0.46
1:L1:314:UNK:O	1:L1:317:UNK:N	2.49	0.46
2:M1:38:UNK:O	2:M1:41:UNK:N	2.49	0.46
2:M1:327:UNK:O	2:M1:330:UNK:N	2.49	0.46
1:L2:108:UNK:O	1:L2:111:UNK:N	2.49	0.46
2:M2:168:UNK:CB	2:M2:174:UNK:CB	2.93	0.46
7:U2:55:UNK:O	7:U2:58:UNK:O	2.34	0.46
10:t2:4:UNK:O	10:t2:7:UNK:N	2.49	0.46
2:M3:87:UNK:HA	2:M3:89:UNK:HA	1.97	0.46
2:M4:124:UNK:O	2:M4:125:UNK:C	2.64	0.46
2:M4:140:UNK:C	2:M4:142:UNK:N	2.74	0.46
3:i4:27:UNK:C	3:i4:28:UNK:O	2.56	0.46
1:L5:108:UNK:O	1:L5:111:UNK:N	2.49	0.46
1:L5:151:UNK:O	1:L5:155:UNK:CA	2.64	0.46
1:L5:316:UNK:O	1:L5:319:UNK:CA	2.64	0.46
10:t5:4:UNK:O	10:t5:7:UNK:N	2.49	0.46
1:L6:271:UNK:O	1:L6:274:UNK:N	2.49	0.46
2:M6:273:UNK:O	2:M6:277:UNK:N	2.48	0.46
2:M1:42:UNK:C	2:M1:44:UNK:N	2.76	0.45
2:M1:118:UNK:O	2:M1:121:UNK:N	2.50	0.45
2:M1:140:UNK:C	2:M1:142:UNK:N	2.74	0.45
5:s1:23:UNK:O	5:s1:26:UNK:N	2.49	0.45
10:t1:4:UNK:O	10:t1:7:UNK:N	2.50	0.45
1:L2:452:UNK:O	1:L2:456:UNK:N	2.48	0.45
1:L3:61:UNK:CA	1:L3:80:UNK:CB	2.93	0.45
2:M3:157:UNK:O	2:M3:160:UNK:N	2.48	0.45
2:M4:32:UNK:C	2:M4:34:UNK:N	2.79	0.45
2:M4:131:UNK:O	2:M4:132:UNK:C	2.63	0.45
5:s5:23:UNK:O	5:s5:26:UNK:N	2.49	0.45
2:M6:87:UNK:HA	2:M6:89:UNK:HA	1.98	0.45
2:M6:168:UNK:CB	2:M6:174:UNK:CB	2.93	0.45
5:s6:23:UNK:O	5:s6:26:UNK:N	2.49	0.45
2:M1:273:UNK:O	2:M1:277:UNK:N	2.48	0.45
2:M2:38:UNK:O	2:M2:41:UNK:N	2.49	0.45
2:M2:131:UNK:O	2:M2:132:UNK:C	2.63	0.45
2:M2:178:UNK:O	2:M2:179:UNK:C	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L3:271:UNK:O	1:L3:274:UNK:N	2.49	0.45
1:L3:452:UNK:O	1:L3:456:UNK:N	2.48	0.45
2:M3:131:UNK:O	2:M3:132:UNK:C	2.63	0.45
1:L4:61:UNK:CA	1:L4:80:UNK:CB	2.93	0.45
1:L4:108:UNK:O	1:L4:111:UNK:N	2.49	0.45
1:L4:239:UNK:C	1:L4:240:UNK:O	2.60	0.45
1:L4:316:UNK:O	1:L4:317:UNK:C	2.63	0.45
2:M4:281:UNK:O	2:M4:284:UNK:C	2.64	0.45
5:p4:8:UNK:O	5:p4:9:UNK:C	2.64	0.45
1:L6:169:UNK:O	1:L6:173:UNK:N	2.49	0.45
1:L6:207:UNK:HA	1:L6:208:UNK:C	2.45	0.45
1:L6:316:UNK:O	1:L6:319:UNK:CA	2.64	0.45
2:M6:118:UNK:O	2:M6:121:UNK:N	2.50	0.45
2:M6:178:UNK:O	2:M6:179:UNK:C	2.63	0.45
2:M6:327:UNK:O	2:M6:330:UNK:N	2.49	0.45
2:M6:432:UNK:O	2:M6:435:UNK:N	2.49	0.45
2:M1:347:UNK:C	2:M1:351:UNK:CB	2.92	0.45
2:M1:348:UNK:CA	2:M1:351:UNK:CB	2.85	0.45
2:M2:87:UNK:HA	2:M2:89:UNK:HA	1.98	0.45
2:M2:159:UNK:O	2:M2:160:UNK:C	2.64	0.45
2:M2:189:UNK:N	2:M2:191:UNK:C	2.75	0.45
7:U3:22:UNK:CA	14:BC:1635:UNK:CB	2.88	0.45
10:t3:4:UNK:O	10:t3:7:UNK:N	2.49	0.45
1:L5:124:UNK:O	1:L5:125:UNK:C	2.63	0.45
1:L6:124:UNK:O	1:L6:125:UNK:C	2.63	0.45
1:L6:151:UNK:O	1:L6:155:UNK:CA	2.64	0.45
10:t6:4:UNK:O	10:t6:7:UNK:N	2.49	0.45
2:M1:432:UNK:O	2:M1:435:UNK:N	2.49	0.45
4:g2:9:UNK:O	4:g2:12:UNK:CB	2.64	0.45
1:L3:124:UNK:O	1:L3:125:UNK:C	2.63	0.45
2:M3:432:UNK:O	2:M3:435:UNK:N	2.49	0.45
4:g3:9:UNK:O	4:g3:12:UNK:CB	2.64	0.45
1:L4:151:UNK:O	1:L4:155:UNK:CA	2.64	0.45
1:L4:169:UNK:O	1:L4:173:UNK:N	2.49	0.45
1:L4:316:UNK:O	1:L4:319:UNK:CA	2.64	0.45
2:M4:432:UNK:O	2:M4:435:UNK:N	2.49	0.45
12:v5:10:UNK:O	12:v5:13:UNK:N	2.49	0.45
1:L6:239:UNK:C	1:L6:240:UNK:O	2.60	0.45
1:L6:316:UNK:O	1:L6:317:UNK:C	2.63	0.45
2:M6:189:UNK:N	2:M6:191:UNK:C	2.75	0.45
2:M1:273:UNK:O	2:M1:276:UNK:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M1:406:UNK:O	2:M1:407:UNK:C	2.64	0.45
7:U1:55:UNK:O	7:U1:58:UNK:O	2.34	0.45
1:L2:29:UNK:CA	1:L2:32:UNK:CB	2.86	0.45
1:L3:207:UNK:HA	1:L3:208:UNK:C	2.45	0.45
2:M3:118:UNK:O	2:M3:121:UNK:N	2.50	0.45
2:M4:225:UNK:CB	2:M4:228:UNK:CB	2.95	0.45
1:L5:29:UNK:CA	1:L5:32:UNK:CB	2.86	0.45
2:M5:432:UNK:O	2:M5:435:UNK:N	2.49	0.45
1:L3:151:UNK:O	1:L3:155:UNK:CA	2.64	0.45
1:L3:165:UNK:HA	1:L3:168:UNK:CB	2.47	0.45
1:L3:297:UNK:CA	1:L3:356:UNK:N	2.73	0.45
12:v3:19:UNK:O	12:v3:23:UNK:N	2.49	0.45
14:BC:1588:UNK:H	14:BF:547:UNK:HA	0.63	0.45
1:L4:246:UNK:O	1:L4:250:UNK:CA	2.65	0.45
2:M4:87:UNK:HA	2:M4:89:UNK:HA	1.97	0.45
2:M4:433:UNK:O	2:M4:434:UNK:C	2.62	0.45
12:v4:19:UNK:O	12:v4:23:UNK:N	2.49	0.45
1:L5:165:UNK:HA	1:L5:168:UNK:CB	2.47	0.45
1:L5:297:UNK:CA	1:L5:356:UNK:N	2.73	0.45
1:L5:314:UNK:O	1:L5:317:UNK:N	2.49	0.45
2:M6:131:UNK:O	2:M6:132:UNK:C	2.63	0.45
1:L1:165:UNK:HA	1:L1:168:UNK:CB	2.47	0.45
1:L1:169:UNK:O	1:L1:173:UNK:N	2.49	0.45
1:L1:288:UNK:CB	1:L1:308:UNK:HA	2.47	0.45
2:M1:61:UNK:N	2:M1:63:UNK:N	2.65	0.45
2:M1:124:UNK:O	2:M1:125:UNK:C	2.64	0.45
2:M1:393:UNK:C	2:M1:395:UNK:N	2.79	0.45
2:M1:433:UNK:O	2:M1:434:UNK:C	2.63	0.45
10:t1:31:UNK:O	10:t1:32:UNK:C	2.65	0.45
1:L2:288:UNK:CB	1:L2:308:UNK:HA	2.47	0.45
2:M2:30:UNK:O	2:M2:33:UNK:N	2.50	0.45
1:L3:169:UNK:O	1:L3:173:UNK:N	2.49	0.45
1:L4:288:UNK:CB	1:L4:308:UNK:HA	2.47	0.45
2:M4:54:UNK:HA	2:M4:55:UNK:HA	1.65	0.45
2:M4:448:UNK:O	2:M4:449:UNK:C	2.61	0.45
3:f4:20:UNK:O	3:f4:24:UNK:CB	2.64	0.45
3:f4:26:UNK:O	3:f4:29:UNK:N	2.50	0.45
14:BD:544:UNK:O	14:BE:1590:UNK:CB	2.64	0.45
14:BE:1625:UNK:C	14:BE:1626:UNK:O	2.65	0.45
1:L6:288:UNK:CB	1:L6:308:UNK:HA	2.47	0.45
7:U6:55:UNK:O	7:U6:58:UNK:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:u6:3:UNK:C	11:u6:5:UNK:N	2.79	0.45
1:L1:239:UNK:C	1:L1:240:UNK:O	2.59	0.45
3:f1:20:UNK:O	3:f1:24:UNK:CB	2.64	0.45
2:M2:32:UNK:C	2:M2:34:UNK:N	2.79	0.45
2:M2:315:UNK:O	2:M2:316:UNK:C	2.64	0.45
7:U3:55:UNK:O	7:U3:58:UNK:O	2.34	0.45
1:L4:165:UNK:HA	1:L4:168:UNK:CB	2.47	0.45
2:M4:114:UNK:CA	2:M4:177:UNK:CB	2.95	0.45
2:M5:393:UNK:C	2:M5:395:UNK:N	2.79	0.45
2:M6:114:UNK:CA	2:M6:177:UNK:CB	2.95	0.45
3:f6:26:UNK:O	3:f6:29:UNK:N	2.50	0.45
5:j6:14:UNK:O	5:j6:17:UNK:N	2.50	0.45
2:M1:178:UNK:O	2:M1:179:UNK:C	2.63	0.45
2:M2:61:UNK:N	2:M2:63:UNK:N	2.65	0.45
2:M2:225:UNK:CB	2:M2:228:UNK:CB	2.95	0.45
1:L3:246:UNK:O	1:L3:250:UNK:CA	2.65	0.45
1:L3:309:UNK:O	1:L3:313:UNK:N	2.50	0.45
2:M3:225:UNK:CB	2:M3:228:UNK:CB	2.95	0.45
10:t3:9:UNK:O	10:t3:10:UNK:C	2.62	0.45
11:u3:3:UNK:C	11:u3:5:UNK:N	2.79	0.45
2:M4:327:UNK:O	2:M4:330:UNK:N	2.49	0.45
11:u4:3:UNK:C	11:u4:5:UNK:N	2.79	0.45
13:w4:3:UNK:O	13:w4:6:UNK:CB	2.65	0.45
2:M5:42:UNK:C	2:M5:44:UNK:N	2.76	0.45
2:M5:87:UNK:HA	2:M5:89:UNK:HA	1.97	0.45
2:M5:178:UNK:O	2:M5:179:UNK:C	2.63	0.45
3:i5:27:UNK:O	3:i5:28:UNK:C	2.65	0.45
14:BF:1625:UNK:C	14:BF:1626:UNK:O	2.65	0.45
1:L1:246:UNK:O	1:L1:250:UNK:CA	2.65	0.45
5:j1:14:UNK:O	5:j1:17:UNK:N	2.50	0.45
8:n1:5:UNK:O	8:n1:8:UNK:CA	2.64	0.45
1:L2:158:UNK:O	1:L2:159:UNK:C	2.64	0.45
1:L2:211:UNK:HA	1:L2:214:UNK:CB	2.47	0.45
2:M2:124:UNK:O	2:M2:125:UNK:C	2.64	0.45
3:f2:26:UNK:O	3:f2:29:UNK:N	2.50	0.45
12:v2:4:UNK:O	12:v2:5:UNK:C	2.65	0.45
2:M3:30:UNK:O	2:M3:33:UNK:N	2.50	0.45
13:w3:3:UNK:O	13:w3:6:UNK:CB	2.65	0.45
2:M4:38:UNK:O	2:M4:41:UNK:N	2.49	0.45
2:M4:42:UNK:C	2:M4:44:UNK:N	2.76	0.45
7:U4:9:UNK:O	7:U4:12:UNK:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:t4:4:UNK:O	10:t4:7:UNK:N	2.49	0.45
14:BD:1625:UNK:C	14:BD:1626:UNK:O	2.65	0.45
1:L5:128:UNK:O	1:L5:129:UNK:C	2.61	0.45
1:L5:246:UNK:O	1:L5:250:UNK:CA	2.65	0.45
2:M5:30:UNK:O	2:M5:33:UNK:N	2.50	0.45
2:M5:124:UNK:O	2:M5:125:UNK:C	2.64	0.45
5:j5:14:UNK:O	5:j5:17:UNK:N	2.50	0.45
4:g6:9:UNK:O	4:g6:12:UNK:CB	2.64	0.45
3:f1:26:UNK:O	3:f1:29:UNK:N	2.50	0.44
1:L2:151:UNK:O	1:L2:155:UNK:CA	2.64	0.44
3:i2:22:UNK:O	3:i2:24:UNK:N	2.51	0.44
11:u2:3:UNK:C	11:u2:5:UNK:N	2.79	0.44
2:M3:175:UNK:C	2:M3:177:UNK:HA	2.47	0.44
2:M4:118:UNK:O	2:M4:121:UNK:N	2.50	0.44
2:M4:178:UNK:O	2:M4:179:UNK:C	2.63	0.44
4:g4:9:UNK:O	4:g4:12:UNK:CB	2.64	0.44
8:n4:5:UNK:O	8:n4:8:UNK:CA	2.64	0.44
14:BD:1614:UNK:C	14:BD:1617:UNK:CA	2.88	0.44
2:M5:54:UNK:HA	2:M5:55:UNK:HA	1.65	0.44
2:M5:61:UNK:N	2:M5:63:UNK:N	2.65	0.44
2:M5:225:UNK:CB	2:M5:228:UNK:CB	2.95	0.44
2:M5:315:UNK:O	2:M5:316:UNK:C	2.64	0.44
2:M6:159:UNK:O	2:M6:160:UNK:C	2.64	0.44
2:M6:225:UNK:CB	2:M6:228:UNK:CB	2.95	0.44
12:v6:4:UNK:O	12:v6:5:UNK:C	2.65	0.44
13:w6:3:UNK:O	13:w6:6:UNK:CB	2.65	0.44
14:BF:1614:UNK:C	14:BF:1617:UNK:CA	2.88	0.44
2:M1:225:UNK:CB	2:M1:228:UNK:CB	2.95	0.44
4:g1:9:UNK:O	4:g1:12:UNK:CB	2.64	0.44
13:w1:3:UNK:O	13:w1:6:UNK:CB	2.65	0.44
3:f2:20:UNK:O	3:f2:24:UNK:CB	2.64	0.44
1:L3:288:UNK:CB	1:L3:308:UNK:HA	2.47	0.44
1:L4:211:UNK:HA	1:L4:214:UNK:CB	2.47	0.44
1:L4:309:UNK:O	1:L4:313:UNK:N	2.50	0.44
2:M4:88:UNK:HA	2:M4:89:UNK:HA	1.84	0.44
2:M5:114:UNK:CA	2:M5:177:UNK:CB	2.95	0.44
2:M5:140:UNK:C	2:M5:142:UNK:N	2.74	0.44
8:n5:5:UNK:O	8:n5:8:UNK:CA	2.64	0.44
1:L6:246:UNK:O	1:L6:250:UNK:CA	2.65	0.44
1:L1:155:UNK:O	1:L1:239:UNK:CB	2.65	0.44
2:M1:62:UNK:N	2:M1:63:UNK:CA	2.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:246:UNK:O	1:L2:250:UNK:CA	2.65	0.44
2:M2:114:UNK:CA	2:M2:177:UNK:CB	2.95	0.44
13:w2:3:UNK:O	13:w2:6:UNK:CB	2.65	0.44
2:M3:433:UNK:O	2:M3:434:UNK:C	2.62	0.44
3:f3:26:UNK:O	3:f3:29:UNK:N	2.50	0.44
5:j3:14:UNK:O	5:j3:17:UNK:N	2.50	0.44
8:n3:5:UNK:O	8:n3:8:UNK:CA	2.65	0.44
12:v3:4:UNK:O	12:v3:5:UNK:C	2.65	0.44
2:M4:91:UNK:O	2:M4:94:UNK:CB	2.66	0.44
2:M4:175:UNK:C	2:M4:177:UNK:HA	2.47	0.44
3:i4:22:UNK:O	3:i4:24:UNK:N	2.51	0.44
2:M5:32:UNK:C	2:M5:34:UNK:N	2.79	0.44
2:M5:118:UNK:O	2:M5:121:UNK:N	2.50	0.44
2:M5:348:UNK:CA	2:M5:351:UNK:CB	2.85	0.44
3:f5:26:UNK:O	3:f5:29:UNK:N	2.50	0.44
3:i5:22:UNK:O	3:i5:24:UNK:N	2.50	0.44
1:L6:165:UNK:HA	1:L6:168:UNK:CB	2.47	0.44
2:M6:32:UNK:C	2:M6:34:UNK:N	2.79	0.44
2:M6:61:UNK:N	2:M6:63:UNK:N	2.65	0.44
2:M6:91:UNK:O	2:M6:94:UNK:CB	2.66	0.44
3:i1:22:UNK:O	3:i1:24:UNK:N	2.51	0.44
7:U1:9:UNK:O	7:U1:12:UNK:N	2.50	0.44
10:t1:6:UNK:C	10:t1:8:UNK:N	2.79	0.44
12:v1:4:UNK:O	12:v1:5:UNK:C	2.65	0.44
1:L2:128:UNK:O	1:L2:129:UNK:C	2.61	0.44
1:L2:165:UNK:HA	1:L2:168:UNK:CB	2.47	0.44
2:M3:42:UNK:C	2:M3:44:UNK:N	2.76	0.44
1:L4:155:UNK:O	1:L4:239:UNK:CB	2.65	0.44
5:j4:14:UNK:O	5:j4:17:UNK:N	2.50	0.44
2:M5:281:UNK:O	2:M5:284:UNK:C	2.64	0.44
1:L6:211:UNK:HA	1:L6:214:UNK:CB	2.48	0.44
3:h1:12:UNK:O	3:h1:15:UNK:N	2.51	0.44
3:i1:25:UNK:O	3:i1:28:UNK:CB	2.66	0.44
10:t1:2:UNK:O	10:t1:5:UNK:CA	2.65	0.44
1:L2:379:UNK:O	1:L2:388:UNK:CB	2.66	0.44
1:L3:155:UNK:O	1:L3:239:UNK:CB	2.65	0.44
1:L3:211:UNK:HA	1:L3:214:UNK:CB	2.48	0.44
2:M3:91:UNK:O	2:M3:94:UNK:CB	2.66	0.44
2:M3:114:UNK:CA	2:M3:177:UNK:CB	2.95	0.44
3:i4:25:UNK:O	3:i4:28:UNK:CB	2.66	0.44
1:L5:211:UNK:HA	1:L5:214:UNK:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U5:55:UNK:O	7:U5:58:UNK:O	2.34	0.44
3:i6:25:UNK:O	3:i6:28:UNK:CB	2.66	0.44
3:i6:27:UNK:C	3:i6:28:UNK:O	2.56	0.44
1:L1:151:UNK:O	1:L1:155:UNK:CA	2.64	0.44
1:L1:379:UNK:O	1:L1:388:UNK:CB	2.66	0.44
2:M1:91:UNK:O	2:M1:94:UNK:CB	2.66	0.44
2:M1:131:UNK:O	2:M1:132:UNK:C	2.63	0.44
2:M1:315:UNK:O	2:M1:316:UNK:C	2.64	0.44
1:L2:155:UNK:O	1:L2:239:UNK:CB	2.65	0.44
2:M2:91:UNK:O	2:M2:94:UNK:CB	2.66	0.44
8:n2:5:UNK:O	8:n2:8:UNK:CA	2.64	0.44
14:BB:1625:UNK:C	14:BB:1626:UNK:O	2.65	0.44
3:i3:22:UNK:O	3:i3:24:UNK:N	2.50	0.44
7:U3:9:UNK:O	7:U3:12:UNK:N	2.50	0.44
2:M5:91:UNK:O	2:M5:94:UNK:CB	2.66	0.44
1:L6:379:UNK:O	1:L6:388:UNK:CB	2.66	0.44
8:n6:5:UNK:O	8:n6:8:UNK:CA	2.64	0.44
1:L1:32:UNK:HA	1:L1:35:UNK:CB	2.48	0.44
1:L1:61:UNK:CA	1:L1:80:UNK:CB	2.93	0.44
1:L1:211:UNK:HA	1:L1:214:UNK:CB	2.47	0.44
2:M1:159:UNK:O	2:M1:160:UNK:C	2.64	0.44
5:p1:8:UNK:O	5:p1:9:UNK:C	2.64	0.44
2:M2:118:UNK:O	2:M2:121:UNK:N	2.50	0.44
3:i2:27:UNK:O	3:i2:28:UNK:C	2.65	0.44
3:i2:27:UNK:C	3:i2:28:UNK:O	2.56	0.44
14:BC:1625:UNK:C	14:BC:1626:UNK:O	2.65	0.44
2:M4:30:UNK:O	2:M4:33:UNK:N	2.50	0.44
10:t4:2:UNK:O	10:t4:5:UNK:CA	2.65	0.44
1:L6:309:UNK:O	1:L6:313:UNK:N	2.50	0.44
2:M6:30:UNK:O	2:M6:33:UNK:N	2.50	0.44
14:BA:1625:UNK:C	14:BA:1626:UNK:O	2.65	0.44
2:M2:22:UNK:HA	2:M2:23:UNK:HA	1.73	0.44
1:L3:379:UNK:O	1:L3:388:UNK:CB	2.66	0.44
2:M3:315:UNK:O	2:M3:316:UNK:C	2.64	0.44
1:L4:124:UNK:O	1:L4:125:UNK:C	2.63	0.44
1:L4:379:UNK:O	1:L4:388:UNK:CB	2.66	0.44
3:h4:12:UNK:O	3:h4:15:UNK:N	2.51	0.44
2:M5:175:UNK:C	2:M5:177:UNK:HA	2.47	0.44
2:M5:433:UNK:O	2:M5:434:UNK:C	2.63	0.44
3:i5:25:UNK:O	3:i5:28:UNK:CB	2.66	0.44
11:u5:3:UNK:C	11:u5:5:UNK:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L6:343:UNK:O	1:L6:347:UNK:N	2.51	0.44
3:i6:22:UNK:O	3:i6:24:UNK:N	2.50	0.44
1:L1:309:UNK:O	1:L1:313:UNK:N	2.50	0.44
1:L3:209:UNK:O	1:L3:210:UNK:C	2.66	0.44
2:M3:61:UNK:N	2:M3:63:UNK:N	2.65	0.44
2:M3:191:UNK:CB	2:M3:192:UNK:CA	2.92	0.44
1:L4:32:UNK:HA	1:L4:35:UNK:CB	2.48	0.44
1:L4:203:UNK:HA	1:L4:204:UNK:HA	1.87	0.44
1:L5:155:UNK:O	1:L5:239:UNK:CB	2.65	0.44
1:L5:309:UNK:O	1:L5:313:UNK:N	2.50	0.44
1:L5:343:UNK:O	1:L5:347:UNK:N	2.51	0.44
3:h5:10:UNK:C	3:h5:12:UNK:N	2.77	0.44
13:w5:3:UNK:O	13:w5:6:UNK:CB	2.65	0.44
1:L6:158:UNK:O	1:L6:159:UNK:C	2.64	0.44
1:L1:250:UNK:O	1:L1:254:UNK:CB	2.66	0.43
2:M3:406:UNK:O	2:M3:407:UNK:C	2.64	0.43
3:h3:12:UNK:O	3:h3:15:UNK:N	2.51	0.43
3:i3:25:UNK:O	3:i3:28:UNK:CB	2.66	0.43
1:L4:77:UNK:CA	1:L4:78:UNK:CB	2.84	0.43
1:L4:250:UNK:O	1:L4:254:UNK:CB	2.66	0.43
1:L5:297:UNK:HA	1:L5:355:UNK:CA	2.48	0.43
3:h5:12:UNK:O	3:h5:15:UNK:N	2.51	0.43
2:M6:433:UNK:O	2:M6:434:UNK:C	2.62	0.43
5:p6:8:UNK:O	5:p6:9:UNK:C	2.64	0.43
1:L1:209:UNK:O	1:L1:210:UNK:C	2.66	0.43
2:M1:30:UNK:O	2:M1:33:UNK:N	2.50	0.43
2:M1:88:UNK:HA	2:M1:89:UNK:HA	1.84	0.43
2:M1:114:UNK:CA	2:M1:177:UNK:CB	2.95	0.43
3:h1:10:UNK:C	3:h1:12:UNK:N	2.77	0.43
1:L2:32:UNK:HA	1:L2:35:UNK:CB	2.48	0.43
2:M2:406:UNK:O	2:M2:407:UNK:C	2.64	0.43
5:j2:14:UNK:O	5:j2:17:UNK:N	2.50	0.43
10:t4:31:UNK:O	10:t4:32:UNK:C	2.65	0.43
2:M5:127:UNK:O	2:M5:128:UNK:C	2.61	0.43
2:M5:131:UNK:O	2:M5:132:UNK:C	2.63	0.43
5:p5:8:UNK:O	5:p5:9:UNK:C	2.64	0.43
5:p5:11:UNK:C	5:p5:13:UNK:N	2.76	0.43
1:L6:155:UNK:O	1:L6:239:UNK:CB	2.65	0.43
7:U6:9:UNK:O	7:U6:12:UNK:N	2.51	0.43
2:M1:175:UNK:C	2:M1:177:UNK:HA	2.47	0.43
1:L2:343:UNK:O	1:L2:347:UNK:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M2:62:UNK:CB	2:M2:65:UNK:N	2.82	0.43
3:i2:25:UNK:O	3:i2:28:UNK:CB	2.66	0.43
7:U2:9:UNK:O	7:U2:12:UNK:N	2.51	0.43
5:p3:11:UNK:C	5:p3:13:UNK:N	2.76	0.43
1:L4:343:UNK:O	1:L4:347:UNK:N	2.51	0.43
2:M4:406:UNK:O	2:M4:407:UNK:C	2.64	0.43
1:L5:32:UNK:HA	1:L5:35:UNK:CB	2.48	0.43
1:L5:288:UNK:CB	1:L5:308:UNK:HA	2.47	0.43
7:U5:9:UNK:O	7:U5:12:UNK:N	2.51	0.43
2:M6:341:UNK:C	2:M6:342:UNK:O	2.56	0.43
5:p6:11:UNK:C	5:p6:13:UNK:N	2.76	0.43
2:M1:54:UNK:HA	2:M1:55:UNK:HA	1.65	0.43
1:L2:309:UNK:O	1:L2:313:UNK:N	2.50	0.43
3:h2:12:UNK:O	3:h2:15:UNK:N	2.51	0.43
5:p2:11:UNK:C	5:p2:13:UNK:N	2.76	0.43
10:t4:9:UNK:O	10:t4:10:UNK:C	2.62	0.43
10:t5:31:UNK:O	10:t5:32:UNK:C	2.65	0.43
1:L6:32:UNK:HA	1:L6:35:UNK:CB	2.48	0.43
1:L6:209:UNK:O	1:L6:210:UNK:C	2.66	0.43
1:L6:250:UNK:O	1:L6:254:UNK:CB	2.66	0.43
3:h6:12:UNK:O	3:h6:15:UNK:N	2.51	0.43
11:u1:3:UNK:C	11:u1:5:UNK:N	2.79	0.43
2:M3:52:UNK:HA	2:M3:53:UNK:HA	1.71	0.43
2:M3:62:UNK:CB	2:M3:65:UNK:N	2.82	0.43
2:M3:159:UNK:O	2:M3:160:UNK:C	2.64	0.43
2:M3:347:UNK:C	2:M3:351:UNK:CB	2.92	0.43
1:L4:108:UNK:O	1:L4:111:UNK:CB	2.67	0.43
2:M4:61:UNK:N	2:M4:63:UNK:N	2.65	0.43
10:t5:2:UNK:O	10:t5:5:UNK:CA	2.65	0.43
1:L6:108:UNK:O	1:L6:111:UNK:CB	2.67	0.43
2:M1:32:UNK:C	2:M1:34:UNK:N	2.79	0.43
2:M2:49:UNK:CA	2:M2:50:UNK:CB	2.84	0.43
2:M4:62:UNK:CB	2:M4:65:UNK:N	2.82	0.43
7:U4:35:UNK:CB	7:U4:39:UNK:N	2.82	0.43
1:L5:209:UNK:O	1:L5:210:UNK:C	2.66	0.43
1:L5:379:UNK:O	1:L5:388:UNK:CB	2.66	0.43
5:s5:21:UNK:O	5:s5:22:UNK:C	2.61	0.43
1:L2:297:UNK:HA	1:L2:355:UNK:CA	2.48	0.43
2:M2:55:UNK:HA	2:M2:56:UNK:HA	1.82	0.43
1:L3:158:UNK:O	1:L3:159:UNK:C	2.64	0.43
2:M3:124:UNK:O	2:M3:125:UNK:C	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:t3:31:UNK:O	10:t3:32:UNK:C	2.65	0.43
1:L4:209:UNK:O	1:L4:210:UNK:C	2.66	0.43
1:L5:250:UNK:O	1:L5:254:UNK:CB	2.67	0.43
7:U5:35:UNK:CB	7:U5:39:UNK:N	2.82	0.43
1:L6:63:UNK:CB	1:L6:78:UNK:CB	2.97	0.43
1:L2:108:UNK:O	1:L2:111:UNK:CB	2.67	0.43
1:L3:343:UNK:O	1:L3:347:UNK:N	2.51	0.43
1:L4:431:UNK:O	1:L4:432:UNK:CB	2.67	0.43
14:BD:1609:UNK:CB	14:BD:1642:UNK:C	2.97	0.43
2:M6:62:UNK:CB	2:M6:65:UNK:N	2.82	0.43
2:M6:315:UNK:O	2:M6:316:UNK:C	2.64	0.43
2:M6:347:UNK:C	2:M6:351:UNK:CB	2.92	0.43
2:M6:406:UNK:O	2:M6:407:UNK:C	2.64	0.43
10:t1:31:UNK:O	10:t1:34:UNK:N	2.52	0.43
7:U2:35:UNK:CB	7:U2:39:UNK:N	2.82	0.43
1:L3:32:UNK:HA	1:L3:35:UNK:CB	2.48	0.43
2:M3:408:UNK:O	2:M3:412:UNK:N	2.52	0.43
10:t3:6:UNK:C	10:t3:8:UNK:N	2.79	0.43
1:L4:82:UNK:O	1:L4:86:UNK:N	2.52	0.43
10:t4:31:UNK:O	10:t4:34:UNK:N	2.52	0.43
1:L5:34:UNK:O	1:L5:37:UNK:N	2.52	0.43
1:L6:34:UNK:O	1:L6:37:UNK:N	2.52	0.43
1:L1:141:UNK:O	1:L1:142:UNK:C	2.67	0.43
1:L2:82:UNK:O	1:L2:86:UNK:N	2.52	0.43
2:M2:408:UNK:O	2:M2:412:UNK:N	2.52	0.43
1:L3:250:UNK:O	1:L3:254:UNK:CB	2.66	0.43
5:p3:8:UNK:O	5:p3:9:UNK:C	2.64	0.43
1:L4:246:UNK:O	1:L4:250:UNK:C	2.65	0.43
2:M5:408:UNK:O	2:M5:412:UNK:N	2.52	0.43
1:L6:141:UNK:O	1:L6:142:UNK:C	2.67	0.43
1:L1:343:UNK:O	1:L1:347:UNK:N	2.51	0.42
2:M1:52:UNK:HA	2:M1:53:UNK:HA	1.71	0.42
14:BA:1609:UNK:CB	14:BA:1642:UNK:C	2.97	0.42
1:L3:203:UNK:HA	1:L3:204:UNK:HA	1.87	0.42
2:M3:22:UNK:CA	2:M3:23:UNK:CB	2.97	0.42
7:U3:35:UNK:CB	7:U3:39:UNK:N	2.82	0.42
2:M4:22:UNK:CA	2:M4:23:UNK:CB	2.97	0.42
2:M4:326:UNK:O	2:M4:327:UNK:C	2.67	0.42
2:M4:393:UNK:C	2:M4:395:UNK:N	2.79	0.42
1:L5:108:UNK:O	1:L5:111:UNK:CB	2.67	0.42
2:M5:62:UNK:CB	2:M5:65:UNK:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M5:164:UNK:O	2:M5:167:UNK:N	2.53	0.42
2:M6:42:UNK:C	2:M6:44:UNK:N	2.76	0.42
3:h6:9:UNK:O	3:h6:12:UNK:CA	2.67	0.42
10:t6:2:UNK:O	10:t6:5:UNK:CA	2.65	0.42
10:t6:31:UNK:O	10:t6:32:UNK:C	2.65	0.42
1:L1:34:UNK:O	1:L1:37:UNK:N	2.52	0.42
1:L1:124:UNK:O	1:L1:125:UNK:C	2.63	0.42
1:L1:140:UNK:O	1:L1:143:UNK:N	2.52	0.42
1:L1:246:UNK:O	1:L1:250:UNK:C	2.65	0.42
2:M1:62:UNK:CB	2:M1:65:UNK:N	2.82	0.42
1:L2:209:UNK:O	1:L2:210:UNK:C	2.66	0.42
1:L2:420:UNK:O	1:L2:423:UNK:N	2.52	0.42
14:BB:1609:UNK:CB	14:BB:1642:UNK:C	2.97	0.42
2:M3:164:UNK:O	2:M3:167:UNK:N	2.53	0.42
1:L4:241:UNK:O	1:L4:242:UNK:C	2.68	0.42
10:t4:6:UNK:C	10:t4:8:UNK:N	2.79	0.42
12:v4:4:UNK:O	12:v4:5:UNK:C	2.65	0.42
10:t5:31:UNK:O	10:t5:34:UNK:N	2.52	0.42
1:L6:140:UNK:O	1:L6:143:UNK:N	2.52	0.42
10:t6:31:UNK:O	10:t6:34:UNK:N	2.52	0.42
1:L2:431:UNK:O	1:L2:432:UNK:CB	2.67	0.42
1:L3:108:UNK:O	1:L3:111:UNK:CB	2.67	0.42
1:L4:158:UNK:O	1:L4:159:UNK:C	2.64	0.42
1:L4:420:UNK:O	1:L4:423:UNK:N	2.52	0.42
1:L5:82:UNK:O	1:L5:86:UNK:N	2.52	0.42
1:L5:241:UNK:O	1:L5:242:UNK:C	2.68	0.42
2:M5:168:UNK:CB	2:M5:174:UNK:CA	2.97	0.42
1:L6:109:UNK:O	1:L6:110:UNK:CB	2.68	0.42
2:M6:54:UNK:HA	2:M6:55:UNK:HA	1.65	0.42
2:M6:175:UNK:C	2:M6:177:UNK:HA	2.47	0.42
2:M6:348:UNK:CA	2:M6:351:UNK:CB	2.85	0.42
14:BF:1609:UNK:CB	14:BF:1642:UNK:C	2.97	0.42
2:M1:168:UNK:CB	2:M1:174:UNK:CA	2.97	0.42
1:L2:109:UNK:O	1:L2:110:UNK:CB	2.67	0.42
1:L3:34:UNK:O	1:L3:37:UNK:N	2.52	0.42
1:L4:63:UNK:CB	1:L4:78:UNK:CB	2.97	0.42
1:L5:140:UNK:O	1:L5:143:UNK:N	2.52	0.42
10:t5:22:UNK:HA	10:t5:25:UNK:CB	2.50	0.42
14:BE:1609:UNK:CB	14:BE:1642:UNK:C	2.97	0.42
14:BE:1614:UNK:C	14:BE:1617:UNK:CA	2.88	0.42
1:L6:369:UNK:O	1:L6:372:UNK:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M6:408:UNK:O	2:M6:412:UNK:N	2.52	0.42
1:L1:158:UNK:O	1:L1:159:UNK:C	2.64	0.42
1:L1:431:UNK:O	1:L1:432:UNK:CB	2.67	0.42
7:U1:11:UNK:O	7:U1:12:UNK:C	2.67	0.42
1:L2:124:UNK:O	1:L2:125:UNK:C	2.63	0.42
1:L2:369:UNK:O	1:L2:372:UNK:N	2.53	0.42
3:h2:10:UNK:C	3:h2:12:UNK:N	2.77	0.42
10:t2:22:UNK:HA	10:t2:25:UNK:CB	2.50	0.42
1:L3:82:UNK:O	1:L3:86:UNK:N	2.52	0.42
1:L3:369:UNK:O	1:L3:372:UNK:N	2.53	0.42
2:M3:54:UNK:HA	2:M3:55:UNK:HA	1.65	0.42
2:M3:55:UNK:HA	2:M3:56:UNK:HA	1.82	0.42
2:M4:52:UNK:HA	2:M4:53:UNK:HA	1.71	0.42
5:s4:26:UNK:O	5:s4:28:UNK:N	2.52	0.42
1:L5:109:UNK:O	1:L5:110:UNK:CB	2.67	0.42
1:L5:128:UNK:O	1:L5:132:UNK:N	2.53	0.42
10:t5:6:UNK:C	10:t5:8:UNK:N	2.79	0.42
2:M1:22:UNK:CA	2:M1:23:UNK:CB	2.97	0.42
2:M2:168:UNK:CB	2:M2:174:UNK:CA	2.97	0.42
7:U2:11:UNK:O	7:U2:12:UNK:C	2.67	0.42
8:n2:45:UNK:O	8:n2:49:UNK:CB	2.68	0.42
10:t2:31:UNK:O	10:t2:34:UNK:N	2.52	0.42
1:L3:63:UNK:CB	1:L3:78:UNK:CB	2.97	0.42
1:L3:109:UNK:O	1:L3:110:UNK:CB	2.67	0.42
1:L3:128:UNK:O	1:L3:132:UNK:N	2.53	0.42
1:L3:420:UNK:O	1:L3:423:UNK:N	2.53	0.42
10:t3:22:UNK:HA	10:t3:25:UNK:CB	2.50	0.42
1:L4:369:UNK:O	1:L4:372:UNK:N	2.53	0.42
2:M5:111:UNK:O	2:M5:112:UNK:CB	2.68	0.42
2:M5:159:UNK:O	2:M5:160:UNK:C	2.64	0.42
7:U6:35:UNK:CB	7:U6:39:UNK:N	2.82	0.42
1:L1:108:UNK:O	1:L1:111:UNK:CB	2.67	0.42
2:M1:369:UNK:O	2:M1:372:UNK:CB	2.68	0.42
2:M1:408:UNK:O	2:M1:412:UNK:N	2.52	0.42
7:U1:35:UNK:CB	7:U1:39:UNK:N	2.82	0.42
1:L2:140:UNK:O	1:L2:143:UNK:N	2.52	0.42
1:L2:241:UNK:O	1:L2:242:UNK:C	2.68	0.42
1:L2:250:UNK:O	1:L2:254:UNK:CB	2.66	0.42
1:L3:241:UNK:O	1:L3:242:UNK:C	2.68	0.42
2:M3:168:UNK:HA	2:M3:174:UNK:HA	2.02	0.42
2:M3:369:UNK:O	2:M3:372:UNK:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:109:UNK:O	1:L4:110:UNK:CB	2.67	0.42
2:M4:179:UNK:O	2:M4:180:UNK:C	2.68	0.42
10:t4:22:UNK:HA	10:t4:25:UNK:CB	2.50	0.42
3:h5:9:UNK:O	3:h5:12:UNK:CA	2.67	0.42
2:M6:22:UNK:CA	2:M6:23:UNK:CB	2.97	0.42
2:M6:124:UNK:O	2:M6:125:UNK:C	2.64	0.42
8:n6:45:UNK:O	8:n6:49:UNK:CB	2.68	0.42
5:s1:26:UNK:O	5:s1:28:UNK:N	2.52	0.42
11:u1:4:UNK:C	11:u1:6:UNK:N	2.82	0.42
1:L2:63:UNK:CB	1:L2:78:UNK:CB	2.97	0.42
2:M2:168:UNK:HA	2:M2:174:UNK:HA	2.02	0.42
2:M2:369:UNK:O	2:M2:372:UNK:CB	2.68	0.42
5:s3:26:UNK:O	5:s3:28:UNK:N	2.52	0.42
1:L4:141:UNK:O	1:L4:142:UNK:C	2.67	0.42
2:M4:113:UNK:CA	2:M4:114:UNK:CB	2.89	0.42
8:n4:45:UNK:O	8:n4:49:UNK:CB	2.68	0.42
1:L5:63:UNK:CB	1:L5:78:UNK:CB	2.97	0.42
2:M5:14:UNK:O	2:M5:15:UNK:C	2.60	0.42
2:M5:55:UNK:HA	2:M5:56:UNK:HA	1.82	0.42
12:v5:4:UNK:O	12:v5:5:UNK:C	2.65	0.42
1:L6:82:UNK:O	1:L6:86:UNK:N	2.52	0.42
1:L6:128:UNK:O	1:L6:132:UNK:N	2.53	0.42
1:L6:420:UNK:O	1:L6:423:UNK:N	2.52	0.42
2:M6:393:UNK:C	2:M6:395:UNK:N	2.79	0.42
1:L1:128:UNK:O	1:L1:132:UNK:N	2.53	0.42
2:M1:50:UNK:O	2:M1:51:UNK:CB	2.68	0.42
1:L2:141:UNK:O	1:L2:142:UNK:C	2.67	0.42
2:M3:113:UNK:CA	2:M3:114:UNK:CB	2.89	0.42
10:t3:3:UNK:O	10:t3:4:UNK:C	2.68	0.42
10:t3:31:UNK:O	10:t3:34:UNK:N	2.52	0.42
14:BC:1609:UNK:CB	14:BC:1642:UNK:C	2.97	0.42
2:M4:111:UNK:O	2:M4:112:UNK:CB	2.68	0.42
2:M4:408:UNK:O	2:M4:412:UNK:N	2.52	0.42
2:M5:179:UNK:O	2:M5:180:UNK:C	2.68	0.42
8:n1:43:UNK:O	8:n1:45:UNK:N	2.53	0.42
1:L2:34:UNK:O	1:L2:37:UNK:N	2.52	0.42
1:L3:141:UNK:O	1:L3:142:UNK:C	2.67	0.42
1:L4:34:UNK:O	1:L4:37:UNK:N	2.52	0.42
1:L4:496:UNK:O	1:L4:497:UNK:C	2.68	0.42
1:L5:420:UNK:O	1:L5:423:UNK:N	2.52	0.42
2:M5:369:UNK:O	2:M5:372:UNK:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L6:431:UNK:O	1:L6:432:UNK:CB	2.67	0.42
10:t6:22:UNK:HA	10:t6:25:UNK:CB	2.50	0.42
1:L1:63:UNK:CB	1:L1:78:UNK:CB	2.97	0.41
1:L1:241:UNK:O	1:L1:242:UNK:C	2.68	0.41
1:L1:274:UNK:O	1:L1:275:UNK:C	2.67	0.41
1:L1:496:UNK:O	1:L1:497:UNK:C	2.68	0.41
2:M1:164:UNK:O	2:M1:167:UNK:N	2.53	0.41
2:M2:54:UNK:HA	2:M2:55:UNK:HA	1.65	0.41
2:M2:111:UNK:O	2:M2:112:UNK:CB	2.68	0.41
3:i2:28:UNK:O	3:i2:29:UNK:CB	2.68	0.41
2:M3:168:UNK:CB	2:M3:174:UNK:CA	2.97	0.41
8:n3:45:UNK:O	8:n3:49:UNK:CB	2.68	0.41
2:M4:164:UNK:O	2:M4:167:UNK:N	2.53	0.41
2:M4:369:UNK:O	2:M4:372:UNK:CB	2.68	0.41
1:L5:141:UNK:O	1:L5:142:UNK:C	2.67	0.41
1:L5:431:UNK:O	1:L5:432:UNK:CB	2.67	0.41
1:L6:65:UNK:CB	1:L6:66:UNK:HA	2.50	0.41
1:L6:496:UNK:O	1:L6:497:UNK:C	2.68	0.41
2:M6:164:UNK:O	2:M6:167:UNK:N	2.52	0.41
11:u6:4:UNK:C	11:u6:6:UNK:N	2.82	0.41
1:L1:82:UNK:O	1:L1:86:UNK:N	2.52	0.41
1:L1:109:UNK:O	1:L1:110:UNK:CB	2.67	0.41
1:L1:369:UNK:O	1:L1:372:UNK:N	2.53	0.41
2:M1:179:UNK:O	2:M1:180:UNK:C	2.68	0.41
2:M1:399:UNK:O	2:M1:403:UNK:N	2.53	0.41
8:n1:45:UNK:O	8:n1:49:UNK:CB	2.68	0.41
1:L2:65:UNK:CB	1:L2:66:UNK:HA	2.50	0.41
1:L2:203:UNK:HA	1:L2:204:UNK:HA	1.88	0.41
2:M2:50:UNK:O	2:M2:51:UNK:CB	2.68	0.41
10:t2:2:UNK:O	10:t2:5:UNK:CA	2.65	0.41
1:L4:140:UNK:O	1:L4:143:UNK:N	2.53	0.41
2:M4:168:UNK:CB	2:M4:174:UNK:CA	2.97	0.41
2:M5:139:UNK:CA	2:M5:140:UNK:CB	2.98	0.41
2:M5:168:UNK:HA	2:M5:174:UNK:HA	2.02	0.41
8:n5:45:UNK:O	8:n5:49:UNK:CB	2.68	0.41
2:M1:275:UNK:HA	2:M1:278:UNK:CB	2.51	0.41
1:L2:182:UNK:O	1:L2:185:UNK:N	2.54	0.41
2:M2:326:UNK:O	2:M2:327:UNK:C	2.67	0.41
1:L3:140:UNK:O	1:L3:143:UNK:N	2.52	0.41
1:L3:274:UNK:O	1:L3:275:UNK:C	2.67	0.41
1:L3:431:UNK:O	1:L3:432:UNK:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L3:496:UNK:O	1:L3:497:UNK:C	2.68	0.41
2:M3:326:UNK:O	2:M3:327:UNK:C	2.67	0.41
2:M3:399:UNK:O	2:M3:403:UNK:N	2.54	0.41
2:M4:275:UNK:HA	2:M4:278:UNK:CB	2.51	0.41
6:l4:23:UNK:O	6:l4:24:UNK:C	2.69	0.41
1:L5:158:UNK:O	1:L5:159:UNK:C	2.64	0.41
2:M5:22:UNK:CA	2:M5:23:UNK:CB	2.97	0.41
11:u5:4:UNK:C	11:u5:6:UNK:N	2.82	0.41
1:L1:182:UNK:O	1:L1:185:UNK:N	2.54	0.41
8:n1:42:UNK:O	8:n1:43:UNK:CB	2.69	0.41
2:M2:399:UNK:O	2:M2:403:UNK:N	2.53	0.41
10:t2:6:UNK:C	10:t2:8:UNK:N	2.79	0.41
2:M3:174:UNK:O	2:M3:175:UNK:C	2.69	0.41
3:i3:28:UNK:O	3:i3:29:UNK:CB	2.68	0.41
1:L5:496:UNK:O	1:L5:497:UNK:C	2.68	0.41
2:M5:50:UNK:O	2:M5:51:UNK:CB	2.68	0.41
2:M5:113:UNK:CA	2:M5:114:UNK:CB	2.89	0.41
6:l5:23:UNK:O	6:l5:24:UNK:C	2.69	0.41
5:s5:13:UNK:O	5:s5:17:UNK:N	2.54	0.41
1:L6:210:UNK:C	1:L6:212:UNK:N	2.82	0.41
2:M6:369:UNK:O	2:M6:372:UNK:CB	2.68	0.41
2:M6:399:UNK:O	2:M6:403:UNK:N	2.53	0.41
3:i6:28:UNK:O	3:i6:29:UNK:CB	2.68	0.41
1:L1:193:UNK:O	1:L1:194:UNK:C	2.69	0.41
2:M2:164:UNK:O	2:M2:167:UNK:N	2.52	0.41
5:s2:13:UNK:O	5:s2:17:UNK:N	2.54	0.41
5:s2:26:UNK:O	5:s2:28:UNK:N	2.52	0.41
1:L3:210:UNK:C	1:L3:212:UNK:N	2.82	0.41
2:M3:88:UNK:HA	2:M3:89:UNK:HA	1.84	0.41
2:M3:179:UNK:O	2:M3:180:UNK:C	2.68	0.41
2:M3:225:UNK:O	2:M3:228:UNK:C	2.69	0.41
2:M3:393:UNK:C	2:M3:395:UNK:N	2.79	0.41
1:L4:418:UNK:O	1:L4:421:UNK:CB	2.69	0.41
2:M4:209:UNK:O	2:M4:210:UNK:C	2.69	0.41
2:M4:225:UNK:O	2:M4:228:UNK:C	2.69	0.41
3:i4:22:UNK:O	3:i4:25:UNK:CB	2.69	0.41
8:n4:43:UNK:O	8:n4:45:UNK:N	2.53	0.41
10:t4:3:UNK:O	10:t4:4:UNK:C	2.68	0.41
1:L5:184:UNK:O	1:L5:188:UNK:N	2.54	0.41
1:L5:203:UNK:HA	1:L5:204:UNK:HA	1.88	0.41
1:L5:369:UNK:O	1:L5:372:UNK:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i5:22:UNK:O	3:i5:25:UNK:CB	2.69	0.41
1:L6:418:UNK:O	1:L6:421:UNK:CB	2.69	0.41
2:M6:88:UNK:HA	2:M6:89:UNK:HA	1.84	0.41
2:M6:111:UNK:O	2:M6:112:UNK:CB	2.68	0.41
2:M6:168:UNK:CB	2:M6:174:UNK:CA	2.97	0.41
5:s6:13:UNK:O	5:s6:17:UNK:N	2.54	0.41
1:L1:420:UNK:O	1:L1:423:UNK:N	2.52	0.41
2:M1:111:UNK:O	2:M1:112:UNK:CB	2.68	0.41
2:M1:168:UNK:HA	2:M1:174:UNK:HA	2.02	0.41
10:t1:22:UNK:HA	10:t1:25:UNK:CB	2.50	0.41
1:L2:128:UNK:O	1:L2:132:UNK:N	2.53	0.41
2:M2:22:UNK:CA	2:M2:23:UNK:CB	2.97	0.41
2:M2:115:UNK:O	2:M2:116:UNK:CB	2.69	0.41
2:M4:50:UNK:O	2:M4:51:UNK:CB	2.68	0.41
2:M4:399:UNK:O	2:M4:403:UNK:N	2.53	0.41
8:n5:43:UNK:O	8:n5:45:UNK:N	2.53	0.41
2:M6:50:UNK:O	2:M6:51:UNK:CB	2.68	0.41
1:L1:192:UNK:O	1:L1:193:UNK:C	2.69	0.41
2:M1:189:UNK:C	2:M1:191:UNK:O	2.69	0.41
3:h1:9:UNK:O	3:h1:12:UNK:CA	2.67	0.41
11:u1:5:UNK:O	11:u1:8:UNK:CB	2.69	0.41
2:M2:327:UNK:O	2:M2:330:UNK:CB	2.69	0.41
2:M2:393:UNK:C	2:M2:395:UNK:N	2.79	0.41
3:i2:22:UNK:O	3:i2:25:UNK:CB	2.69	0.41
1:L3:418:UNK:O	1:L3:421:UNK:CB	2.69	0.41
2:M3:327:UNK:O	2:M3:330:UNK:CB	2.69	0.41
3:i3:22:UNK:O	3:i3:25:UNK:CB	2.69	0.41
1:L4:128:UNK:O	1:L4:132:UNK:N	2.53	0.41
1:L4:182:UNK:O	1:L4:185:UNK:N	2.54	0.41
2:M5:209:UNK:O	2:M5:210:UNK:C	2.69	0.41
2:M6:133:UNK:O	2:M6:224:UNK:CB	2.69	0.41
2:M6:179:UNK:O	2:M6:180:UNK:C	2.68	0.41
2:M6:209:UNK:O	2:M6:210:UNK:C	2.69	0.41
2:M6:275:UNK:HA	2:M6:278:UNK:CB	2.51	0.41
2:M6:327:UNK:O	2:M6:330:UNK:CB	2.69	0.41
2:M1:29:UNK:O	2:M1:30:UNK:C	2.69	0.41
3:i1:22:UNK:O	3:i1:25:UNK:CB	2.69	0.41
1:L2:191:UNK:O	1:L2:192:UNK:CB	2.69	0.41
1:L2:496:UNK:O	1:L2:497:UNK:C	2.68	0.41
2:M2:139:UNK:CA	2:M2:140:UNK:CB	2.98	0.41
8:n2:42:UNK:O	8:n2:43:UNK:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:t2:31:UNK:O	10:t2:32:UNK:C	2.65	0.41
2:M3:50:UNK:O	2:M3:51:UNK:CB	2.68	0.41
2:M3:186:UNK:O	2:M3:253:UNK:CB	2.69	0.41
1:L4:184:UNK:O	1:L4:188:UNK:N	2.54	0.41
2:M4:382:UNK:O	2:M4:383:UNK:C	2.69	0.41
3:i4:28:UNK:O	3:i4:29:UNK:CB	2.68	0.41
1:L5:167:UNK:O	1:L5:170:UNK:CB	2.69	0.41
2:M5:52:UNK:HA	2:M5:53:UNK:HA	1.71	0.41
2:M5:327:UNK:O	2:M5:330:UNK:CB	2.69	0.41
2:M5:399:UNK:O	2:M5:403:UNK:N	2.53	0.41
1:L6:184:UNK:O	1:L6:188:UNK:N	2.54	0.41
3:h6:10:UNK:C	3:h6:12:UNK:N	2.77	0.41
8:n6:8:UNK:O	8:n6:11:UNK:CB	2.69	0.41
1:L1:275:UNK:O	1:L1:278:UNK:N	2.54	0.41
2:M1:133:UNK:O	2:M1:224:UNK:CB	2.69	0.41
2:M1:186:UNK:O	2:M1:253:UNK:CB	2.69	0.41
2:M1:225:UNK:O	2:M1:228:UNK:C	2.69	0.41
3:i1:28:UNK:O	3:i1:29:UNK:CB	2.68	0.41
8:n1:8:UNK:O	8:n1:11:UNK:CB	2.69	0.41
1:L2:161:UNK:CB	1:L2:163:UNK:N	2.84	0.41
1:L2:246:UNK:O	1:L2:250:UNK:C	2.66	0.41
1:L2:275:UNK:O	1:L2:278:UNK:N	2.54	0.41
2:M2:133:UNK:O	2:M2:224:UNK:CB	2.69	0.41
2:M2:209:UNK:O	2:M2:210:UNK:C	2.69	0.41
2:M2:345:UNK:O	2:M2:346:UNK:CB	2.69	0.41
6:l2:23:UNK:O	6:l2:24:UNK:C	2.69	0.41
1:L3:161:UNK:CB	1:L3:163:UNK:N	2.84	0.41
1:L3:182:UNK:O	1:L3:183:UNK:C	2.69	0.41
1:L3:184:UNK:O	1:L3:188:UNK:N	2.54	0.41
1:L3:297:UNK:CA	1:L3:355:UNK:HA	2.50	0.41
1:L3:298:UNK:O	1:L3:301:UNK:CB	2.69	0.41
2:M3:189:UNK:C	2:M3:191:UNK:O	2.69	0.41
2:M3:209:UNK:O	2:M3:210:UNK:C	2.69	0.41
2:M3:382:UNK:O	2:M3:385:UNK:CB	2.69	0.41
5:s3:13:UNK:O	5:s3:17:UNK:N	2.54	0.41
1:L4:65:UNK:CB	1:L4:66:UNK:HA	2.50	0.41
1:L4:167:UNK:O	1:L4:170:UNK:CB	2.69	0.41
2:M4:115:UNK:O	2:M4:116:UNK:CB	2.69	0.41
2:M4:163:UNK:O	2:M4:164:UNK:C	2.69	0.41
2:M4:240:UNK:O	2:M4:241:UNK:C	2.69	0.41
2:M4:327:UNK:O	2:M4:330:UNK:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i4:27:UNK:O	3:i4:28:UNK:C	2.65	0.41
8:n4:8:UNK:O	8:n4:11:UNK:CB	2.69	0.41
8:n4:42:UNK:O	8:n4:43:UNK:CB	2.69	0.41
11:u4:4:UNK:C	11:u4:6:UNK:N	2.82	0.41
11:u4:5:UNK:O	11:u4:8:UNK:CB	2.69	0.41
1:L5:275:UNK:O	1:L5:278:UNK:N	2.54	0.41
1:L5:298:UNK:O	1:L5:301:UNK:CB	2.69	0.41
2:M5:225:UNK:O	2:M5:228:UNK:C	2.69	0.41
2:M5:382:UNK:O	2:M5:383:UNK:C	2.69	0.41
7:U5:11:UNK:O	7:U5:12:UNK:C	2.67	0.41
8:n5:8:UNK:O	8:n5:11:UNK:CB	2.69	0.41
1:L6:275:UNK:O	1:L6:278:UNK:N	2.54	0.41
1:L6:297:UNK:HA	1:L6:355:UNK:CA	2.48	0.41
1:L6:298:UNK:O	1:L6:301:UNK:CB	2.69	0.41
2:M6:49:UNK:CA	2:M6:50:UNK:CB	2.84	0.41
2:M6:381:UNK:O	2:M6:382:UNK:C	2.67	0.41
11:u6:5:UNK:O	11:u6:8:UNK:CB	2.69	0.41
1:L1:297:UNK:HA	1:L1:355:UNK:CA	2.48	0.41
2:M1:167:UNK:O	2:M1:171:UNK:CB	2.70	0.41
2:M1:172:UNK:O	2:M1:173:UNK:CB	2.69	0.41
14:BA:1601:UNK:C	14:BA:1605:UNK:N	2.74	0.41
1:L2:167:UNK:O	1:L2:170:UNK:CB	2.69	0.41
1:L2:274:UNK:O	1:L2:275:UNK:C	2.67	0.41
1:L2:298:UNK:O	1:L2:301:UNK:CB	2.69	0.41
2:M2:179:UNK:O	2:M2:180:UNK:C	2.68	0.41
2:M2:240:UNK:O	2:M2:241:UNK:C	2.69	0.41
2:M2:251:UNK:O	2:M2:252:UNK:CB	2.69	0.41
2:M2:275:UNK:HA	2:M2:278:UNK:CB	2.51	0.41
3:h2:9:UNK:O	3:h2:12:UNK:CA	2.67	0.41
1:L3:67:UNK:O	1:L3:68:UNK:CB	2.69	0.41
1:L3:182:UNK:O	1:L3:185:UNK:N	2.54	0.41
2:M3:167:UNK:O	2:M3:171:UNK:CB	2.69	0.41
2:M3:367:UNK:O	2:M3:368:UNK:CB	2.69	0.41
2:M3:382:UNK:O	2:M3:383:UNK:C	2.69	0.41
7:U3:36:UNK:O	7:U3:42:UNK:CB	2.69	0.41
8:n3:8:UNK:O	8:n3:11:UNK:CB	2.69	0.41
10:t3:28:UNK:O	10:t3:29:UNK:C	2.69	0.41
1:L4:192:UNK:O	1:L4:193:UNK:C	2.69	0.41
1:L4:275:UNK:O	1:L4:278:UNK:N	2.54	0.41
2:M4:57:UNK:O	2:M4:58:UNK:CB	2.70	0.41
2:M4:189:UNK:C	2:M4:191:UNK:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M4:322:UNK:O	2:M4:323:UNK:C	2.69	0.41
5:s4:13:UNK:O	5:s4:17:UNK:N	2.54	0.41
1:L5:65:UNK:CB	1:L5:66:UNK:HA	2.50	0.41
1:L5:67:UNK:O	1:L5:68:UNK:CB	2.69	0.41
1:L5:386:UNK:O	1:L5:387:UNK:CB	2.69	0.41
2:M5:326:UNK:O	2:M5:327:UNK:C	2.67	0.41
5:s5:12:UNK:O	5:s5:13:UNK:C	2.69	0.41
1:L6:182:UNK:O	1:L6:185:UNK:N	2.54	0.41
2:M6:139:UNK:CA	2:M6:140:UNK:CB	2.98	0.41
2:M6:345:UNK:O	2:M6:346:UNK:CB	2.69	0.41
10:t6:33:UNK:O	10:t6:36:UNK:CA	2.69	0.41
1:L1:67:UNK:O	1:L1:68:UNK:CB	2.69	0.40
2:M1:115:UNK:O	2:M1:116:UNK:CB	2.69	0.40
2:M1:327:UNK:O	2:M1:330:UNK:CB	2.69	0.40
2:M1:382:UNK:O	2:M1:385:UNK:CB	2.69	0.40
1:L2:418:UNK:O	1:L2:421:UNK:CB	2.69	0.40
2:M2:108:UNK:O	2:M2:111:UNK:CB	2.69	0.40
2:M2:186:UNK:O	2:M2:253:UNK:CB	2.69	0.40
8:n2:8:UNK:O	8:n2:11:UNK:CB	2.69	0.40
10:t2:3:UNK:O	10:t2:4:UNK:C	2.68	0.40
1:L3:114:UNK:O	1:L3:115:UNK:C	2.70	0.40
2:M3:133:UNK:O	2:M3:224:UNK:CB	2.69	0.40
6:l3:23:UNK:O	6:l3:24:UNK:C	2.69	0.40
11:u3:4:UNK:C	11:u3:6:UNK:N	2.82	0.40
1:L4:274:UNK:O	1:L4:275:UNK:C	2.67	0.40
2:M4:382:UNK:O	2:M4:385:UNK:CB	2.69	0.40
7:U4:11:UNK:O	7:U4:12:UNK:C	2.67	0.40
1:L5:114:UNK:O	1:L5:115:UNK:C	2.70	0.40
2:M5:115:UNK:O	2:M5:116:UNK:CB	2.69	0.40
2:M5:322:UNK:O	2:M5:323:UNK:C	2.69	0.40
1:L6:114:UNK:O	1:L6:115:UNK:C	2.69	0.40
1:L6:241:UNK:O	1:L6:242:UNK:C	2.68	0.40
2:M6:7:UNK:O	2:M6:8:UNK:C	2.70	0.40
2:M6:367:UNK:O	2:M6:368:UNK:CB	2.69	0.40
1:L1:34:UNK:O	1:L1:37:UNK:CB	2.69	0.40
1:L1:65:UNK:CB	1:L1:66:UNK:HA	2.50	0.40
1:L1:182:UNK:O	1:L1:183:UNK:C	2.69	0.40
1:L1:418:UNK:O	1:L1:421:UNK:CB	2.69	0.40
3:i1:27:UNK:O	3:i1:28:UNK:C	2.65	0.40
6:l1:23:UNK:O	6:l1:24:UNK:C	2.69	0.40
2:M2:225:UNK:O	2:M2:228:UNK:C	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M2:367:UNK:O	2:M2:368:UNK:CB	2.69	0.40
8:n2:43:UNK:O	8:n2:45:UNK:N	2.53	0.40
11:u2:5:UNK:O	11:u2:8:UNK:CB	2.69	0.40
1:L3:189:UNK:O	1:L3:194:UNK:CA	2.69	0.40
1:L4:165:UNK:O	1:L4:168:UNK:N	2.55	0.40
2:M4:87:UNK:CB	2:M4:88:UNK:CA	2.95	0.40
2:M4:159:UNK:O	2:M4:160:UNK:C	2.64	0.40
4:g4:20:UNK:C	4:g4:22:UNK:N	2.84	0.40
1:L5:34:UNK:O	1:L5:37:UNK:CB	2.69	0.40
1:L5:418:UNK:O	1:L5:421:UNK:CB	2.69	0.40
2:M5:382:UNK:O	2:M5:385:UNK:CB	2.69	0.40
4:g5:20:UNK:C	4:g5:22:UNK:N	2.84	0.40
10:t5:4:UNK:O	10:t5:5:UNK:C	2.70	0.40
1:L6:111:UNK:O	1:L6:114:UNK:CB	2.70	0.40
2:M6:115:UNK:O	2:M6:116:UNK:CB	2.69	0.40
2:M6:189:UNK:C	2:M6:191:UNK:O	2.69	0.40
10:t6:6:UNK:C	10:t6:8:UNK:N	2.79	0.40
1:L1:191:UNK:O	1:L1:192:UNK:CB	2.69	0.40
10:t1:19:UNK:O	10:t1:20:UNK:C	2.70	0.40
1:L2:34:UNK:O	1:L2:37:UNK:CB	2.69	0.40
1:L2:184:UNK:O	1:L2:188:UNK:N	2.54	0.40
1:L2:189:UNK:O	1:L2:194:UNK:CA	2.69	0.40
2:M2:213:UNK:O	2:M2:214:UNK:C	2.70	0.40
1:L3:167:UNK:O	1:L3:170:UNK:CB	2.69	0.40
1:L3:246:UNK:O	1:L3:250:UNK:C	2.66	0.40
1:L3:275:UNK:O	1:L3:278:UNK:N	2.54	0.40
2:M3:111:UNK:O	2:M3:112:UNK:CB	2.68	0.40
2:M3:345:UNK:O	2:M3:346:UNK:CB	2.69	0.40
3:h3:9:UNK:O	3:h3:12:UNK:CA	2.67	0.40
3:h3:10:UNK:C	3:h3:12:UNK:N	2.77	0.40
5:s3:12:UNK:O	5:s3:13:UNK:C	2.69	0.40
1:L4:65:UNK:CB	1:L4:67:UNK:CA	2.94	0.40
1:L4:111:UNK:O	1:L4:114:UNK:CB	2.70	0.40
1:L4:161:UNK:CB	1:L4:163:UNK:N	2.84	0.40
1:L4:185:UNK:O	1:L4:188:UNK:CB	2.70	0.40
1:L4:298:UNK:O	1:L4:301:UNK:CB	2.69	0.40
2:M4:106:UNK:O	2:M4:109:UNK:CB	2.70	0.40
2:M4:186:UNK:O	2:M4:253:UNK:CB	2.69	0.40
2:M4:309:UNK:O	2:M4:310:UNK:C	2.70	0.40
1:L5:111:UNK:O	1:L5:114:UNK:CB	2.70	0.40
1:L5:161:UNK:CB	1:L5:163:UNK:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:165:UNK:O	1:L5:168:UNK:N	2.55	0.40
2:M5:186:UNK:O	2:M5:253:UNK:CB	2.69	0.40
2:M5:251:UNK:O	2:M5:252:UNK:CB	2.69	0.40
8:n5:57:UNK:O	8:n5:58:UNK:CB	2.70	0.40
5:s5:26:UNK:O	5:s5:28:UNK:N	2.52	0.40
2:M6:20:UNK:O	2:M6:21:UNK:CB	2.70	0.40
2:M6:108:UNK:O	2:M6:111:UNK:CB	2.69	0.40
2:M6:168:UNK:HA	2:M6:174:UNK:HA	2.02	0.40
1:L1:298:UNK:O	1:L1:299:UNK:C	2.70	0.40
1:L1:298:UNK:O	1:L1:301:UNK:CB	2.69	0.40
2:M1:106:UNK:O	2:M1:109:UNK:CB	2.70	0.40
2:M1:213:UNK:O	2:M1:214:UNK:C	2.70	0.40
2:M1:370:UNK:O	2:M1:371:UNK:C	2.70	0.40
7:U1:48:UNK:O	7:U1:52:UNK:N	2.55	0.40
5:s1:13:UNK:O	5:s1:17:UNK:N	2.54	0.40
10:t1:4:UNK:O	10:t1:5:UNK:C	2.70	0.40
1:L2:67:UNK:O	1:L2:68:UNK:CB	2.69	0.40
1:L2:296:UNK:O	1:L2:356:UNK:CB	2.70	0.40
2:M2:20:UNK:O	2:M2:21:UNK:CB	2.70	0.40
2:M2:175:UNK:C	2:M2:177:UNK:HA	2.47	0.40
2:M2:189:UNK:C	2:M2:191:UNK:O	2.69	0.40
1:L3:111:UNK:O	1:L3:114:UNK:CB	2.70	0.40
1:L3:185:UNK:O	1:L3:188:UNK:CB	2.70	0.40
2:M3:66:UNK:O	2:M3:67:UNK:C	2.70	0.40
2:M3:172:UNK:O	2:M3:173:UNK:CB	2.69	0.40
8:n3:42:UNK:O	8:n3:43:UNK:CB	2.69	0.40
1:L4:182:UNK:O	1:L4:183:UNK:C	2.69	0.40
1:L4:297:UNK:HA	1:L4:355:UNK:CA	2.48	0.40
1:L4:386:UNK:O	1:L4:387:UNK:CB	2.69	0.40
2:M4:172:UNK:O	2:M4:173:UNK:CB	2.69	0.40
2:M4:174:UNK:O	2:M4:175:UNK:C	2.69	0.40
8:n4:57:UNK:O	8:n4:58:UNK:CB	2.70	0.40
1:L5:182:UNK:O	1:L5:183:UNK:C	2.69	0.40
1:L5:191:UNK:O	1:L5:192:UNK:CB	2.69	0.40
2:M5:20:UNK:O	2:M5:21:UNK:CB	2.70	0.40
2:M5:167:UNK:O	2:M5:171:UNK:CB	2.70	0.40
7:U5:48:UNK:O	7:U5:52:UNK:N	2.55	0.40
11:u5:5:UNK:O	11:u5:8:UNK:CB	2.69	0.40
1:L6:154:UNK:O	1:L6:155:UNK:C	2.70	0.40
2:M6:57:UNK:O	2:M6:58:UNK:CB	2.69	0.40
2:M6:106:UNK:O	2:M6:109:UNK:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M6:167:UNK:O	2:M6:171:UNK:CB	2.69	0.40
2:M6:172:UNK:O	2:M6:173:UNK:CB	2.69	0.40
2:M6:382:UNK:O	2:M6:385:UNK:CB	2.69	0.40
3:i6:22:UNK:O	3:i6:25:UNK:CB	2.69	0.40
3:i6:27:UNK:O	3:i6:28:UNK:C	2.65	0.40
1:L1:111:UNK:O	1:L1:114:UNK:CB	2.70	0.40
1:L1:154:UNK:O	1:L1:155:UNK:C	2.70	0.40
1:L1:185:UNK:O	1:L1:188:UNK:CB	2.70	0.40
2:M1:60:UNK:C	2:M1:62:UNK:O	2.69	0.40
2:M1:243:UNK:O	2:M1:244:UNK:C	2.70	0.40
1:L2:114:UNK:O	1:L2:115:UNK:C	2.69	0.40
1:L2:136:UNK:O	1:L2:137:UNK:C	2.70	0.40
1:L2:224:UNK:O	1:L2:225:UNK:CB	2.70	0.40
2:M2:29:UNK:O	2:M2:30:UNK:C	2.68	0.40
2:M2:66:UNK:O	2:M2:67:UNK:C	2.70	0.40
2:M2:146:UNK:O	2:M2:147:UNK:C	2.70	0.40
2:M2:160:UNK:O	2:M2:161:UNK:C	2.70	0.40
1:L3:34:UNK:O	1:L3:37:UNK:CB	2.69	0.40
2:M3:115:UNK:O	2:M3:116:UNK:CB	2.69	0.40
2:M3:157:UNK:O	2:M3:158:UNK:C	2.70	0.40
2:M3:392:UNK:O	2:M3:393:UNK:C	2.70	0.40
7:U3:48:UNK:O	7:U3:52:UNK:N	2.55	0.40
10:t3:33:UNK:O	10:t3:36:UNK:CA	2.69	0.40
11:u3:5:UNK:O	11:u3:8:UNK:CB	2.69	0.40
2:M4:133:UNK:O	2:M4:224:UNK:CB	2.69	0.40
5:s4:18:UNK:O	5:s4:19:UNK:C	2.70	0.40
10:t4:33:UNK:O	10:t4:36:UNK:CA	2.69	0.40
10:t4:54:UNK:O	10:t4:55:UNK:C	2.70	0.40
1:L5:182:UNK:O	1:L5:185:UNK:N	2.54	0.40
1:L5:192:UNK:O	1:L5:193:UNK:C	2.69	0.40
2:M5:66:UNK:O	2:M5:67:UNK:C	2.70	0.40
2:M5:106:UNK:O	2:M5:109:UNK:CB	2.70	0.40
2:M5:189:UNK:C	2:M5:191:UNK:O	2.69	0.40
8:n5:42:UNK:O	8:n5:43:UNK:CB	2.69	0.40
14:BE:1634:UNK:O	14:BE:1637:UNK:C	2.70	0.40
1:L6:67:UNK:O	1:L6:68:UNK:CB	2.69	0.40
1:L6:185:UNK:O	1:L6:188:UNK:CB	2.70	0.40
2:M6:66:UNK:O	2:M6:67:UNK:C	2.70	0.40
2:M6:225:UNK:O	2:M6:228:UNK:C	2.69	0.40
2:M6:251:UNK:O	2:M6:252:UNK:CB	2.69	0.40
7:U6:36:UNK:O	7:U6:42:UNK:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s6:26:UNK:O	5:s6:28:UNK:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	BA	9
14	BB	9
14	BC	9
14	BD	9
14	BE	9
14	BF	9
1	L4	4
1	L1	4
1	L2	4
1	L3	4
1	L5	4
1	L6	4
2	M1	1
2	M2	1
2	M3	1
2	M4	1
2	M5	1
2	M6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	563:UNK	C	571:UNK	N	83.40
1	BB	563:UNK	C	571:UNK	N	83.40
1	BC	563:UNK	C	571:UNK	N	83.40
1	BD	563:UNK	C	571:UNK	N	83.40
1	BE	563:UNK	C	571:UNK	N	83.40
1	BF	563:UNK	C	571:UNK	N	83.40
1	BA	1649:UNK	C	1651:UNK	N	70.87
1	BB	1649:UNK	C	1651:UNK	N	70.87
1	BC	1649:UNK	C	1651:UNK	N	70.87
1	BD	1649:UNK	C	1651:UNK	N	70.87
1	BE	1649:UNK	C	1651:UNK	N	70.87
1	BF	1649:UNK	C	1651:UNK	N	70.87
1	BA	1668:UNK	C	1669:UNK	N	66.49
1	BB	1668:UNK	C	1669:UNK	N	66.49
1	BC	1668:UNK	C	1669:UNK	N	66.49
1	BD	1668:UNK	C	1669:UNK	N	66.49
1	BE	1668:UNK	C	1669:UNK	N	66.49
1	BF	1668:UNK	C	1669:UNK	N	66.49
1	BA	587:UNK	C	1588:UNK	N	45.91
1	BB	587:UNK	C	1588:UNK	N	45.91
1	BC	587:UNK	C	1588:UNK	N	45.91
1	BD	587:UNK	C	1588:UNK	N	45.91

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BE	587:UNK	C	1588:UNK	N	45.91
1	BF	587:UNK	C	1588:UNK	N	45.91
1	BA	547:UNK	C	548:UNK	N	31.70
1	BB	547:UNK	C	548:UNK	N	31.70
1	BC	547:UNK	C	548:UNK	N	31.70
1	BD	547:UNK	C	548:UNK	N	31.70
1	BE	547:UNK	C	548:UNK	N	31.70
1	BF	547:UNK	C	548:UNK	N	31.70
1	M1	415:UNK	C	430:UNK	N	22.06
1	M2	415:UNK	C	430:UNK	N	22.06
1	M3	415:UNK	C	430:UNK	N	22.06
1	M4	415:UNK	C	430:UNK	N	22.06
1	M5	415:UNK	C	430:UNK	N	22.06
1	M6	415:UNK	C	430:UNK	N	22.06
1	L4	400:UNK	C	408:UNK	N	14.38
1	L1	400:UNK	C	408:UNK	N	14.37
1	L2	400:UNK	C	408:UNK	N	14.37
1	L3	400:UNK	C	408:UNK	N	14.37
1	L5	400:UNK	C	408:UNK	N	14.37
1	L6	400:UNK	C	408:UNK	N	14.37
1	BA	1626:UNK	C	1632:UNK	N	14.07
1	BB	1626:UNK	C	1632:UNK	N	14.07
1	BC	1626:UNK	C	1632:UNK	N	14.07
1	BD	1626:UNK	C	1632:UNK	N	14.07
1	BE	1626:UNK	C	1632:UNK	N	14.07
1	BF	1626:UNK	C	1632:UNK	N	14.07
1	L1	22:UNK	C	28:UNK	N	11.17
1	L2	22:UNK	C	28:UNK	N	11.17
1	L3	22:UNK	C	28:UNK	N	11.17
1	L4	22:UNK	C	28:UNK	N	11.17
1	L5	22:UNK	C	28:UNK	N	11.17
1	L6	22:UNK	C	28:UNK	N	11.17
1	L1	358:UNK	C	363:UNK	N	8.92
1	L2	358:UNK	C	363:UNK	N	8.92
1	L3	358:UNK	C	363:UNK	N	8.92
1	L4	358:UNK	C	363:UNK	N	8.92
1	L5	358:UNK	C	363:UNK	N	8.92
1	L6	358:UNK	C	363:UNK	N	8.92
1	BA	1659:UNK	C	1660:UNK	N	7.79
1	BB	1659:UNK	C	1660:UNK	N	7.79
1	BC	1659:UNK	C	1660:UNK	N	7.79
1	BD	1659:UNK	C	1660:UNK	N	7.79

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BE	1659:UNK	C	1660:UNK	N	7.79
1	BF	1659:UNK	C	1660:UNK	N	7.79
1	BA	1639:UNK	C	1642:UNK	N	5.24
1	BB	1639:UNK	C	1642:UNK	N	5.24
1	BC	1639:UNK	C	1642:UNK	N	5.24
1	BD	1639:UNK	C	1642:UNK	N	5.24
1	BE	1639:UNK	C	1642:UNK	N	5.24
1	BF	1639:UNK	C	1642:UNK	N	5.24
1	L1	486:UNK	C	487:UNK	N	3.84
1	L2	486:UNK	C	487:UNK	N	3.84
1	L3	486:UNK	C	487:UNK	N	3.84
1	L4	486:UNK	C	487:UNK	N	3.84
1	L5	486:UNK	C	487:UNK	N	3.84
1	L6	486:UNK	C	487:UNK	N	3.84
1	BA	533:UNK	C	534:UNK	N	0.91
1	BB	533:UNK	C	534:UNK	N	0.91
1	BC	533:UNK	C	534:UNK	N	0.91
1	BD	533:UNK	C	534:UNK	N	0.91
1	BE	533:UNK	C	534:UNK	N	0.91
1	BF	533:UNK	C	534:UNK	N	0.91

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L1	0/606	-	-	-	-
1	L2	0/606	-	-	-	-
1	L3	0/606	-	-	-	-
1	L4	0/606	-	-	-	-
1	L5	0/606	-	-	-	-
1	L6	0/606	-	-	-	-
2	M1	0/459	-	-	-	-
2	M2	0/459	-	-	-	-
2	M3	0/459	-	-	-	-
2	M4	0/459	-	-	-	-
2	M5	0/459	-	-	-	-
2	M6	0/459	-	-	-	-
3	f1	0/30	-	-	-	-
3	f2	0/30	-	-	-	-
3	f3	0/30	-	-	-	-
3	f4	0/30	-	-	-	-
3	f5	0/30	-	-	-	-
3	f6	0/30	-	-	-	-
3	h1	0/30	-	-	-	-
3	h2	0/30	-	-	-	-
3	h3	0/30	-	-	-	-
3	h4	0/30	-	-	-	-
3	h5	0/30	-	-	-	-
3	h6	0/30	-	-	-	-
3	i1	0/30	-	-	-	-
3	i2	0/30	-	-	-	-
3	i3	0/30	-	-	-	-
3	i4	0/30	-	-	-	-
3	i5	0/30	-	-	-	-
3	i6	0/30	-	-	-	-
4	g1	0/22	-	-	-	-
4	g2	0/22	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	g3	0/22	-	-	-	-
4	g4	0/22	-	-	-	-
4	g5	0/22	-	-	-	-
4	g6	0/22	-	-	-	-
5	j1	0/28	-	-	-	-
5	j2	0/28	-	-	-	-
5	j3	0/28	-	-	-	-
5	j4	0/28	-	-	-	-
5	j5	0/28	-	-	-	-
5	j6	0/28	-	-	-	-
5	k1	0/28	-	-	-	-
5	k2	0/28	-	-	-	-
5	k3	0/28	-	-	-	-
5	k4	0/28	-	-	-	-
5	k5	0/28	-	-	-	-
5	k6	0/28	-	-	-	-
5	p1	0/28	-	-	-	-
5	p2	0/28	-	-	-	-
5	p3	0/28	-	-	-	-
5	p4	0/28	-	-	-	-
5	p5	0/28	-	-	-	-
5	p6	0/28	-	-	-	-
5	s1	0/28	-	-	-	-
5	s2	0/28	-	-	-	-
5	s3	0/28	-	-	-	-
5	s4	0/28	-	-	-	-
5	s5	0/28	-	-	-	-
5	s6	0/28	-	-	-	-
6	l1	0/13	-	-	-	-
6	l2	0/13	-	-	-	-
6	l3	0/13	-	-	-	-
6	l4	0/13	-	-	-	-
6	l5	0/13	-	-	-	-
6	l6	0/13	-	-	-	-
7	U1	0/88	-	-	-	-
7	U2	0/88	-	-	-	-
7	U3	0/88	-	-	-	-
7	U4	0/88	-	-	-	-
7	U5	0/88	-	-	-	-
7	U6	0/88	-	-	-	-
8	n1	0/59	-	-	-	-
8	n2	0/59	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
8	n3	0/59	-	-	-	-
8	n4	0/59	-	-	-	-
8	n5	0/59	-	-	-	-
8	n6	0/59	-	-	-	-
9	o1	0/21	-	-	-	-
9	o2	0/21	-	-	-	-
9	o3	0/21	-	-	-	-
9	o4	0/21	-	-	-	-
9	o5	0/21	-	-	-	-
9	o6	0/21	-	-	-	-
10	t1	0/57	-	-	-	-
10	t2	0/57	-	-	-	-
10	t3	0/57	-	-	-	-
10	t4	0/57	-	-	-	-
10	t5	0/57	-	-	-	-
10	t6	0/57	-	-	-	-
11	u1	0/15	-	-	-	-
11	u2	0/15	-	-	-	-
11	u3	0/15	-	-	-	-
11	u4	0/15	-	-	-	-
11	u5	0/15	-	-	-	-
11	u6	0/15	-	-	-	-
12	v1	0/32	-	-	-	-
12	v2	0/32	-	-	-	-
12	v3	0/32	-	-	-	-
12	v4	0/32	-	-	-	-
12	v5	0/32	-	-	-	-
12	v6	0/32	-	-	-	-
13	w1	0/27	-	-	-	-
13	w2	0/27	-	-	-	-
13	w3	0/27	-	-	-	-
13	w4	0/27	-	-	-	-
13	w5	0/27	-	-	-	-
13	w6	0/27	-	-	-	-
14	BA	0/146	-	-	-	-
14	BB	0/146	-	-	-	-
14	BC	0/146	-	-	-	-
14	BD	0/146	-	-	-	-
14	BE	0/146	-	-	-	-
14	BF	0/146	-	-	-	-
All	All	0/10482	-	-	-	-

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.